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SUPPORTING INFORMATION

Supporting Information
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Thieme

Copper-Catalyzed Aerobic C–H Trifluoromethylation of Phenanthrolines

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Supporting Material

A. General Information

General Procedures. All reactions were performed in oven-dried or flame-dried round-bottom flasks and vials. Stainless steel syringes and cannula were used to transfer air- and moisture-sensitive liquids. Flash chromatography was performed using silica gel 60 (230-400 mesh) from Sigma–Aldrich.

Materials. Commercial reagents were purchased from Sigma Aldrich, Fluka, EM Science, and Lancaster and used as received. All solvents were used after being freshly distilled unless otherwise noted.

Instrumentation. Proton nuclear magnetic resonance (^{1}HNMR) spectra， carbon nuclear magnetic resonance (^{13}C NMR) spectra and fluorine nuclear magnetic resonance (^{19}F NMR) were recorded on Bruker UltraShield-400 (400 MHz). Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to the NMR solvent residual peak ($CHCl_3$: δ 7.26). Chemical shifts for carbons are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the NMR solvent ($CDCl_3$: δ 77.0). Chemical shifts for fluorine are reported in parts per million downfield and are referenced to the fluorine resonances of $CFCl_3$. Data are represented as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz), and integration.

The mass spectroscopic data were obtained at the Georgia State University mass spectrometry facility using a Micromass Platform II single quadruple instrument. Infrared (IR) spectra were obtained using a Perkin Elmer Spectrum 100 FT-IR spectrometer.

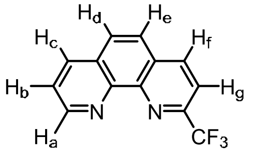
Abbreviations used: EtOH–ethanol, EtOAc–ethyl acetate, THF–tetrahydrofuran, MeOH–methanol, Et_2O–diethyl ether, CH_2Cl_2–dichloromethane, TEA–triethylamine, MeCN–acetonitrile, MS–molecular sieves, TLC–thin layer chromatography.

B. Procedure for the Copper-Catalyzed Aerobic C−H Trifluoromethylation of Phenanthrolines

a. General Procedures:

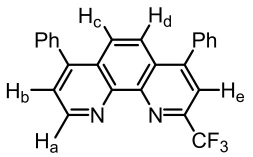
To a mixture of 1, 10-phenanthroline **1** (36 mg, 0.2 mmol), Cu (OAc)$_2$ (7.4 mg, 0.04 mmol), KOAc (9.8mg, 0.1 mmol) and AcOH (6.0 µL, 0.1 mmol) in toluene (4.0 mL), TMSCF$_3$ (30 µL, 0.2 mmol) was added at room temperature under O$_2$ atmosphere. The reaction mixture was stirred 40 °C for 3 hours. Another portion of TMSCF$_3$ (30 µL, 0.2 mmol) was added and continue stirring at 40 °C. The reaction was monitored by TLC. After the starting material was completely consumed, the reaction was quenched by H$_2$O and extracted with EtOAc (3x 4 mL). The combined organic layer was washed by brine, dried over Na$_2$SO$_4$ and concentrated *in vacuo*. The product was isolated through a silica gel flash column (40% EtOAc in hexanes) as a white foam (41 mg, 80% yield).

1,10-Phenanthroline, 4,7-diphenyl-1,10-phenanthroline and 4,7-dimethyl-1,10-phenanthroline are commercially available and are used directly without further purification. 3-Phenyl-1,10-phenanthroline,[1] 3,8-diphenyl-1,10-phenanthroline,[2] and 5-nitro-1,10-phenanthroline were synthesized according to literature procedures.[3]



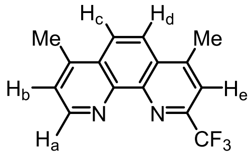
2

2-(Trifluoromethyl)-1,10-phenanthroline (2) : Compound **2** was isolated through a silica gel flash column (80% yield) as a white foam. ^{1}H NMR (400 MHz, CDCl$_3$, ppm): δ 9.24 (s, H$_a$), 8.38 (d, J = 8.4 Hz, H$_f$), 8.23 (d, J = 8.6 Hz, H$_c$), 7.93 (d, J = 8.4 Hz, H$_g$), 7.85, 7.78 (d, J = 8.8Hz, H$_{d\,\&}$ H$_e$), 7.65 (m, H$_b$); ^{13}C NMR (100 MHz, CDCl$_3$, ppm): δ 151.06, 147.7 (q, J = 35.0 Hz), 145.72, 145.56, 137.83, 136.09, 129.76, 129.10, 128.79, 125.70, 123.59, 124.30 (q, J = 273 Hz), 119.00; ^{19}F NMR (377 MHz, CDCl$_3$, ppm): δ -66.59 (s, 3F). IR ν_{max} (neat)/cm^{-1}: 3696, 2967, 2217, 1595, 1337, 1112, 851, 746. HRMS (ESI, m/z): calcd for $C_{13}H_8N_2F_3^+$ [M+H$^+$]: 249.0640, found: 249.0642.



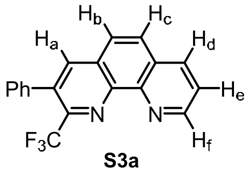
S1a

4,7-Diphenyl-2-(trifluoromethyl)-1,10-phenanthroline (S1a): Compound **S1a** was isolated through a silica gel flash column as an off-white foam (92% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.31 (d, J = 4.4 Hz, H_a), 7.96, 7.87 (d, J = 9.6 Hz, H_c & H_d), 7.93 (s, H_e), 7.61 (d, J = 4.4 Hz, H_b), 7.53-7.50 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 150.6, 150.5, 148.6, 147.8, 147.4, 147.1, 146.7, 146.4, 146.4, 137.4, 136.9, 129.5, 129.0, 128.8, 128.6, 127.7, 126.9, 126.3, 125.8, 124.0, 123.4, 123.1, 120.3, 119.5, 119.49, 117.6; ^{19}F NMR (376 MHz, $CDCl_3$, ppm): δ -66.40 (s, 3F); IR ν_{max} (neat)/cm^{-1} : 3058, 2212, 1375, 1118, 1072, 838, 726; HRMS (ESI) calcd for $C_{25}H_{16}N_3F_3$ $[M+H]^+$: 401.1266 , found 401.1251.



S2a

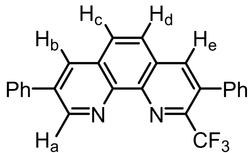
4,7-Dimethyl-2-(trifluoromethyl)-1,10-phenanthroline (S2a): Compound **S2a** was isolated through a silica gel flash column as a white foam (61% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.13 (d, J = 4.4 Hz, H_a), 8.15, 8.05 (d, J = 9.2 Hz, H_c & H_d), 7.81 (s, H_e), 7.50 (d, J = 4.0 Hz, H_b), 2.88 (s, 3H), 2.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 150.8, 147.3, 146.7, 146.0, 145.7, 144.4, 129.0, 128.4, 124.6, 124.4, 121.4, 120.0, 119.9, 19.5, 19.0; ^{19}F NMR (376 MHz, $CDCl_3$, ppm): δ -66.59 (s, 3F); IR ν_{max} (neat)/cm^{-1} : 3701, 2953, 1397, 1275, 1228, 1130, 1033, 877, 739; HRMS (ESI) calcd for $C_{15}H_{12}N_3F_3$ $[M+H]^+$: 277.0953 , found 277.0948.



S3a

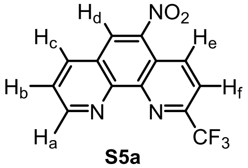
3-Phenyl-2-(trifluoromethyl)-1,10-phenanthroline (S3a): Compound **S3a** was isolated through a silica gel flash column as a white foam (64% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.31

(d, *J* = 3.6 Hz H_f), 8.31 (d, *J* = 8.0 Hz, H_d), 8.28 (s, H_a), 7.95, 7.85 (d, H_b & H_c, *J* = 8.8 Hz), 7.71 (dd, *J* = 8.0 Hz, 4.4 Hz, H_e), 7.32-7.49 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 151.3, 145.9, 143.9, 139.9, 137.2, 136.3, 136.0, 129.4, 129.2, 129.1, 128.5, 128.4, 126.0, 125.6, 123.6, 123.3, 120.5, 115.8; ^{19}F NMR (376 MHz, $CDCl_3$, ppm): δ -66.53 (s, 3F); IR ν_{max} (neat)/cm^{-1} : 3048, 2923, 1721, 1557, 1314, 1125, 930, 697; HRMS (ESI) calcd for $C_{19}H_{12}N_2F_3$ $[M+H]^+$: 325.0953 , found 325.0941.



S4a

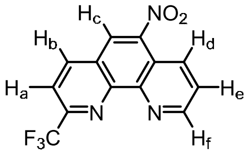
3,8-Diphenyl-2-(trifluoromethyl)-1,10-phenanthroline (S4a): Compound **S4a** was isolated through a silica gel flash column as a white foam (52% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.56 (s, H_a), 8.45 (s, H_e), 8.29 (s, H_b), 8.01, 7.88 (d, *J* = 8.8 Hz, $H_{c\,\&}\,H_d$), 7.80 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.2 Hz, 2H), 7.261-7.259 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 150.4, 144.7, 139.9, 137.3, 137.2, 136.4, 135.8, 133.6, 129.5, 129.4, 129.3, 129.2, 129.0, 128.6, 128.4, 128.2, 127.6, 126.1; ^{19}F NMR (376 MHz, $CDCl_3$, ppm): δ -60.45 (s, 3F); IR ν_{max} (neat)/cm^{-1} : 3706, 2923, 1418, 1315, 1180, 1070, 931, 119, 699; HRMS (ESI) calcd for $C_{25}H_{16}N_2F_3$ $[M+H]^+$: 401.1266 , found 401.1251.



S5a

5-Nitro-2-(trifluoromethyl)-1,10-phenanthroline (S5a)[5]: Compound **S5a** was isolated through a silica gel flash column as a light yellow foam (17% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.47 (d, *J* = 4.4 Hz, H_a), 9.31 (d, *J* = 8.8 Hz, H_f), 8.85 (s, H_d), 8.49 (d, *J* = 8.0 Hz, H_c), 8.18 (d, *J* = 8.8 Hz, H_e), 7.85 (dd, *J* = 8.0 Hz, 4.4 Hz, H_b); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 152.4, 151.1, 150.8, 1150.4, 147.0, 146.0, 140.0, 132.5, 126.8, 125.0, 124.1, 122.5, 121.5; ^{19}F NMR

(376 MHz, $CDCl_3$, ppm): δ -67.00 (s, 3F); IR ν_{max} (neat)/cm^{-1} : 3083, 2921, 1734, 1525, 1337, 1147, 1071, 846, 781; HRMS (ESI) calcd for $C_{13}H_7N_3O_2F_3$ $[M+H]^+$: 294.0490, found 294.0492.

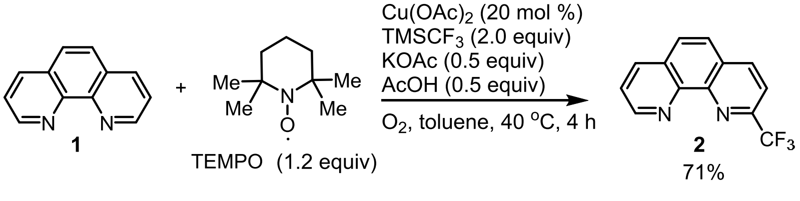


S5b

6-Nitro-2-(trifluoromethyl)-1,10-phenanthroline (S5b): Compound **S5b** was isolated through a silica gel flash column as a light yellow foam (54% yield). ^1H NMR (400 MHz, $CDCl_3$, ppm): δ 9.41 (d, J = 4.0 Hz, H_f), 8.99 (d, J = 8.8 Hz, H_d), 8.70 (s, H_c), 8.66 (d, J = 8.4 Hz, H_b), 8.13 (d, J = 8.0 Hz, H_a), 7.88 (dd, J = 8.8 Hz, 4.0 Hz, H_e); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 154.5, 149.4, 149.1, 147.4, 145.8, 143.6, 138.1, 135.1, 127.9, 126.1, 125.0, 122.6, 122.4, 120.6, 120.55, 119.8; ^{19}F NMR (376 MHz, $CDCl_3$, ppm): δ -67.05 (s, 3F); IR ν_{max} (neat)/cm^{-1} : 3053, 2921, 1623, 1529, 1333, 1176, 1071, 913, 843, 768; HRMS (ESI) calcd for $C_{13}H_7N_3O_2F_3$ $[M+H]^+$: 294.0490 , found 294.0493.

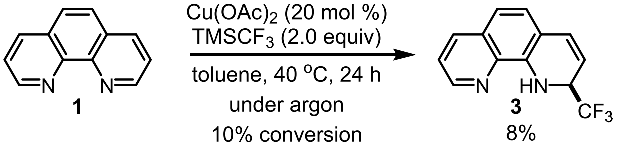
b. Control Experiments to Probe for a Possible Mechanism

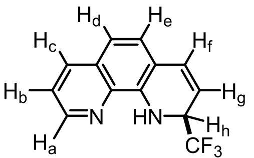
Scheme S1. A control experiment in the presence of TEMPO



Procedure: To a mixture of 1, 10-phenanthroline **1** (18 mg, 0.1 mmol), Cu $(OAc)_2$ (3.7 mg, 0.02 mmol), KOAc (4.9 mg, 0.05 mmol), HOAc (3.0 μL, 0.05 mmol) and TEMPO (19 mg, 0.12 mmol, 1.2 equiv) in toluene (2.0 mL), $TMSCF_3$ (15 μL, 0.1 mmol) was added at room temperature under O_2 atmosphere. The reaction mixture was allowed to stir at 40 °C for 3 hours. Another portion of $TMSCF_3$ (15 μL, 0.1 mmol) was added and continue stirring at 40 °C The reaction was monitored by TLC. After the starting material was completely consumed, the reaction was quenched by H_2O and extracted with EtOAc (3x 4 mL). The desired product was purified according to the general procedure.

Scheme S2. Control experiment under argon affords 1, 2-dihydrophenanthroline

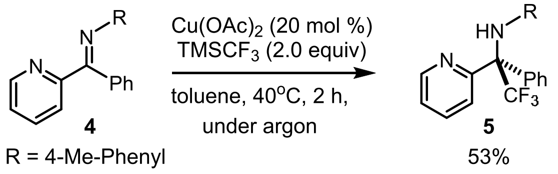


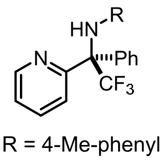


3

2-(Trifluoromethyl)-1,2-dihydro-1,10-phenanthroline (3)[4]: Compound **3** was isolated through a silica gel flash column as colorless oil (8% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.72 (d, J = 3.2 Hz, H_a), 8.01 (d, J = 8.4 Hz, H_c), 7.34 (q, J = 4.0 Hz, H_b), 7.14, 7.04 (d, J = 8.0 Hz, H_d & H_e), 6.77 (d, J = 10.0 Hz, H_f), 6.41 (s, NH), 5.63 (td, J = 7.6 Hz, 2.0 Hz, H_g), 5.12 (m, H_h); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 147.9, 138.5, 136.6, 136.0, 129.0, 126.0, 125.2, 123.7 (q, J = 264 Hz), 121.6, 115.1, 114.2, 113.4, 55.0 (q, J = 31 Hz); ^{19}F NMR (377 MHz, $CDCl_3$, ppm): δ -81.24 (d, J = 7.5 Hz). IR ν_{max} (neat)/cm^{-1}: 3672, 2928, 2513, 2159, 2029, 1977, 1384, 1120, 1067. HRMS (ESI, m/z): calcd for $C_{13}H_{10}N_2F_3^+$ [M+H$^+$]: 251.0796, found: 251.0791.

Scheme S3. Imine trifluoromethylation without the quinolinyl directing group





R = 4-Me-phenyl

5

4-Methyl-*N*-(2,2,2-trifluoro-1-phenyl-1-(pyridin-2-yl)ethyl)aniline (5)[4]: Compound **5** was isolated through a silica gel flash column as a white foam (53% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.75 (d, J = 4.4 Hz, 1H), 7.67 (d, J = 6.8 Hz, 2H), 7.61 (t, J = 7.6 Hz, 1H), 7.47-7.43 (m, 3H), 7.33-7.30 (m, 1H), 7.19 (s, 1H), 7.06 (d, J = 8.0 Hz, 1H), 6.90 (d, J = 8.0 Hz, 2H), 6.53 (d, J = 8.0 Hz, 2H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.47, 147.21, 141.66, 137.79, 136.57, 128.99, 128.77, 128.42, 128.40, 128.16, 127.22, 126.30 (q, J = 290 Hz), 125.03, 123.26, 116.30, 68.79 (q, J = 26 Hz), 20.28. ^{19}F NMR (377 MHz, $CDCl_3$, ppm): δ -66.88. . IR ν_{max} (neat)/cm^{-1}: 3346, 1615, 1516, 1257, 1146, 932, 699. HRMS (ESI, m/z): calcd for $C_{20}H_{18}F_3N_2$ [M+H$^+$]: 343.1422; Found: 343.1419.

C. References

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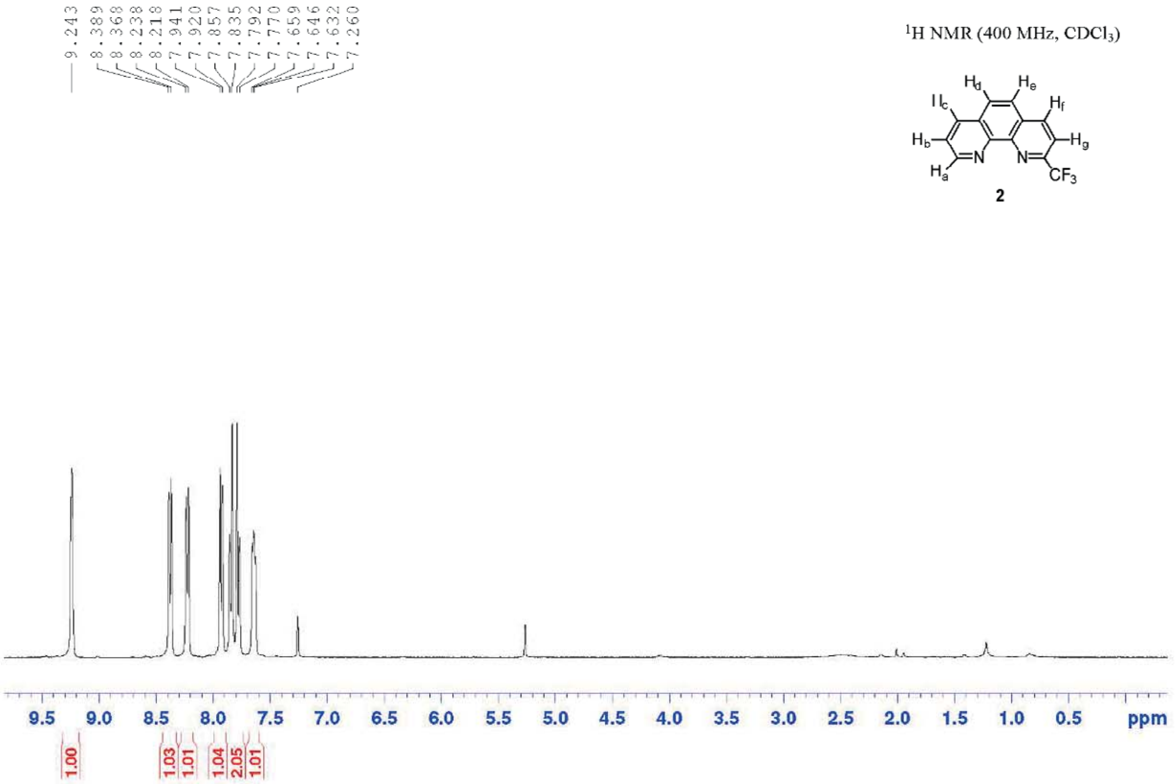
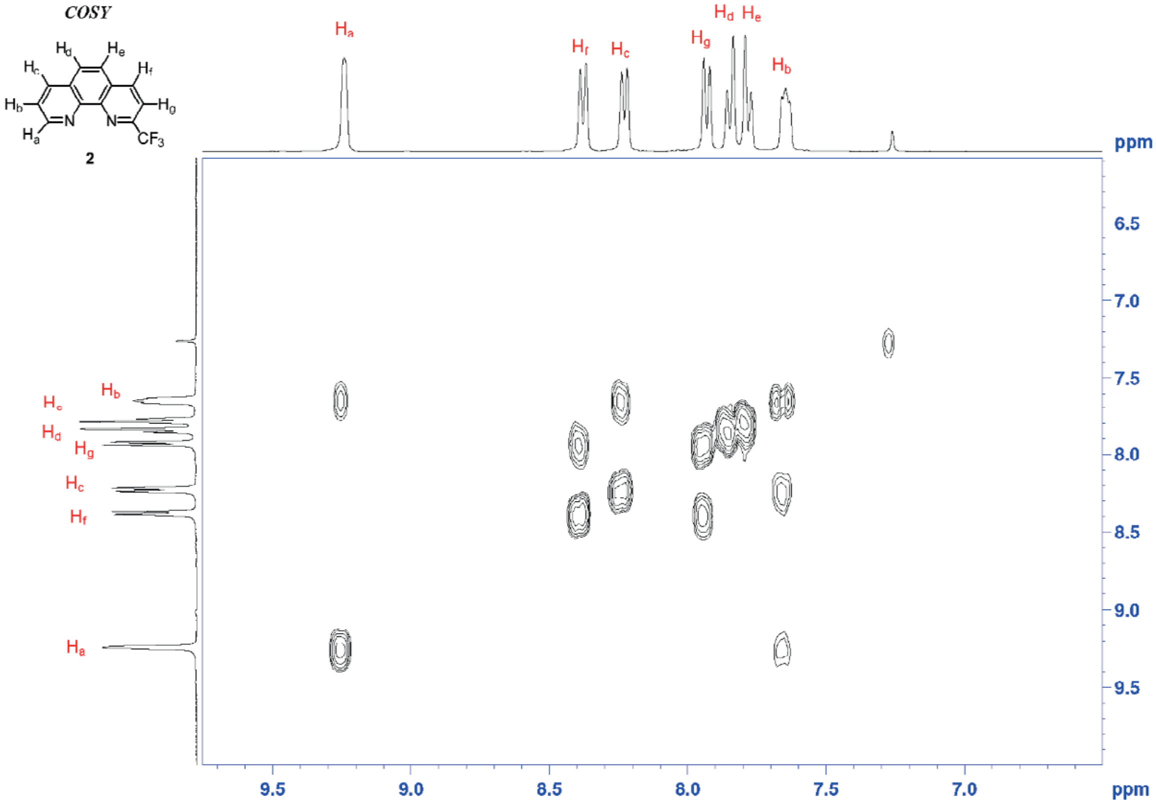
5. Compounds **S5a** and **S5b** were distinguished from each other by NOESY analysis.

D. NMR Spectra


^{1}H NMR (400 MHz, CDCl$_3$)

2

COSY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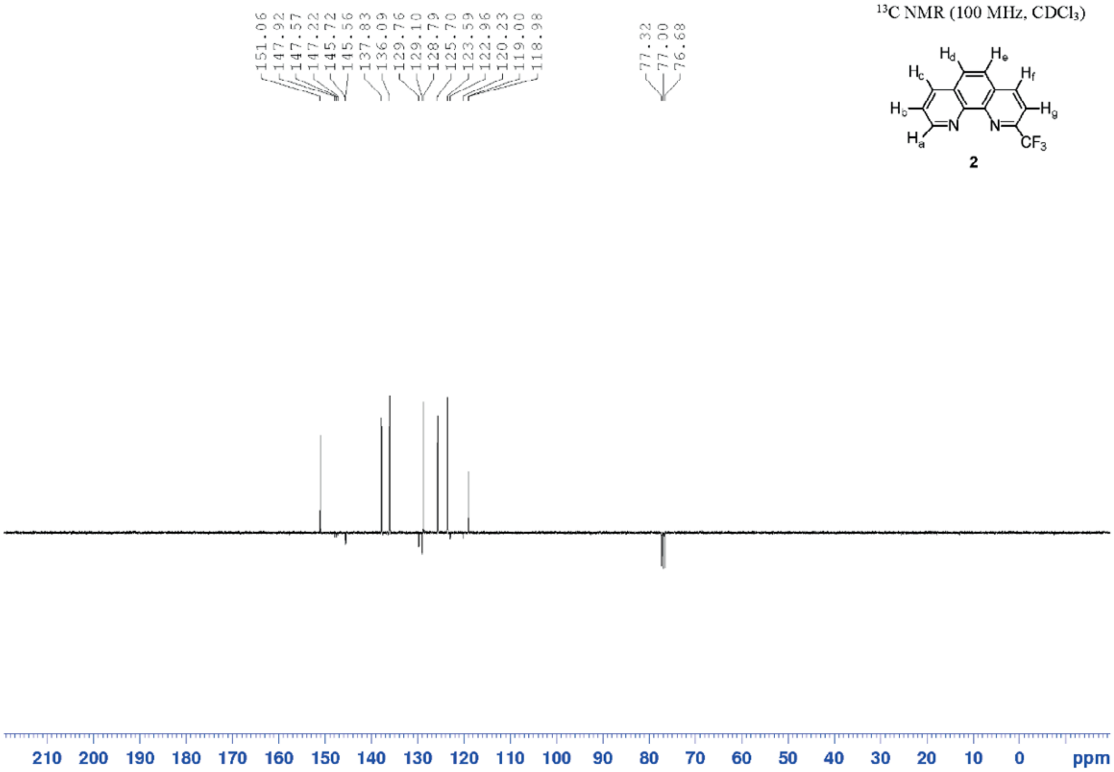
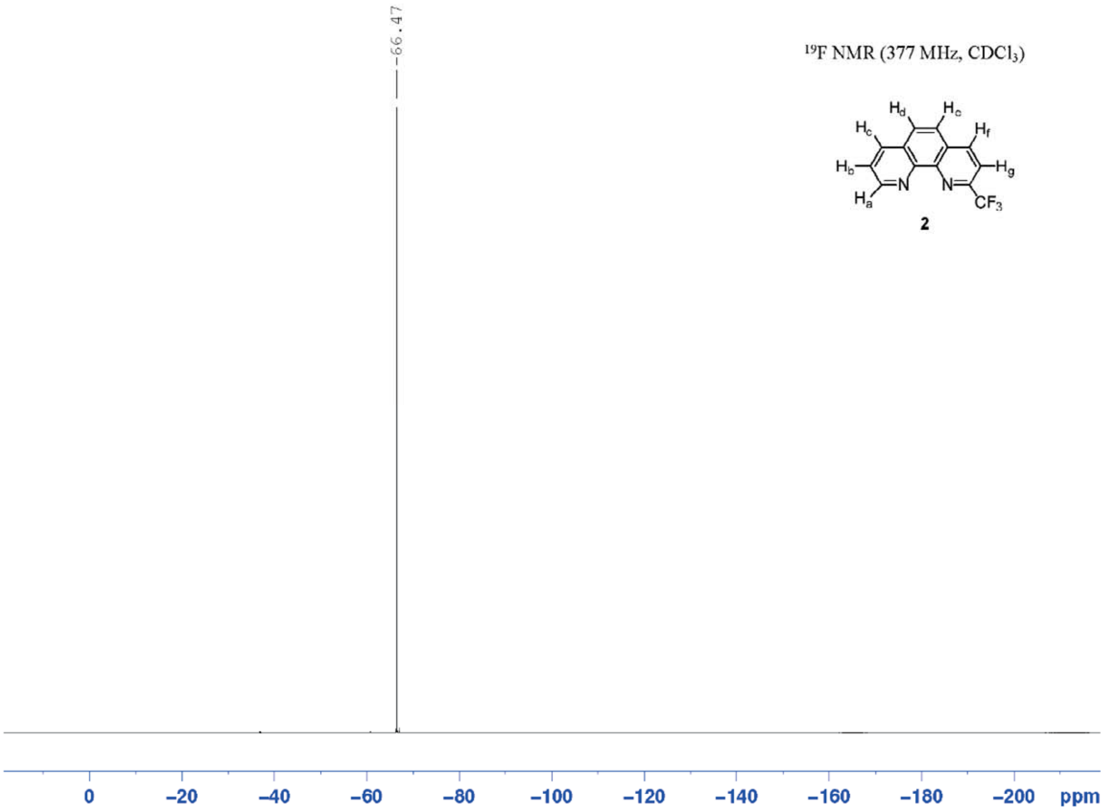
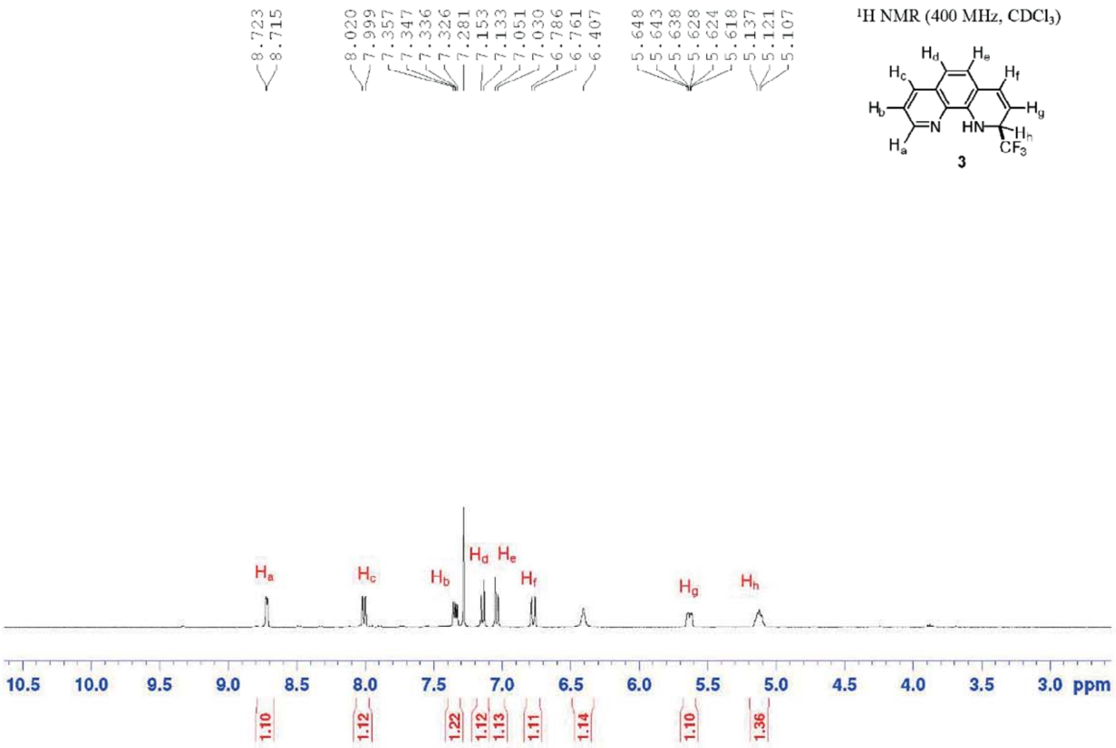
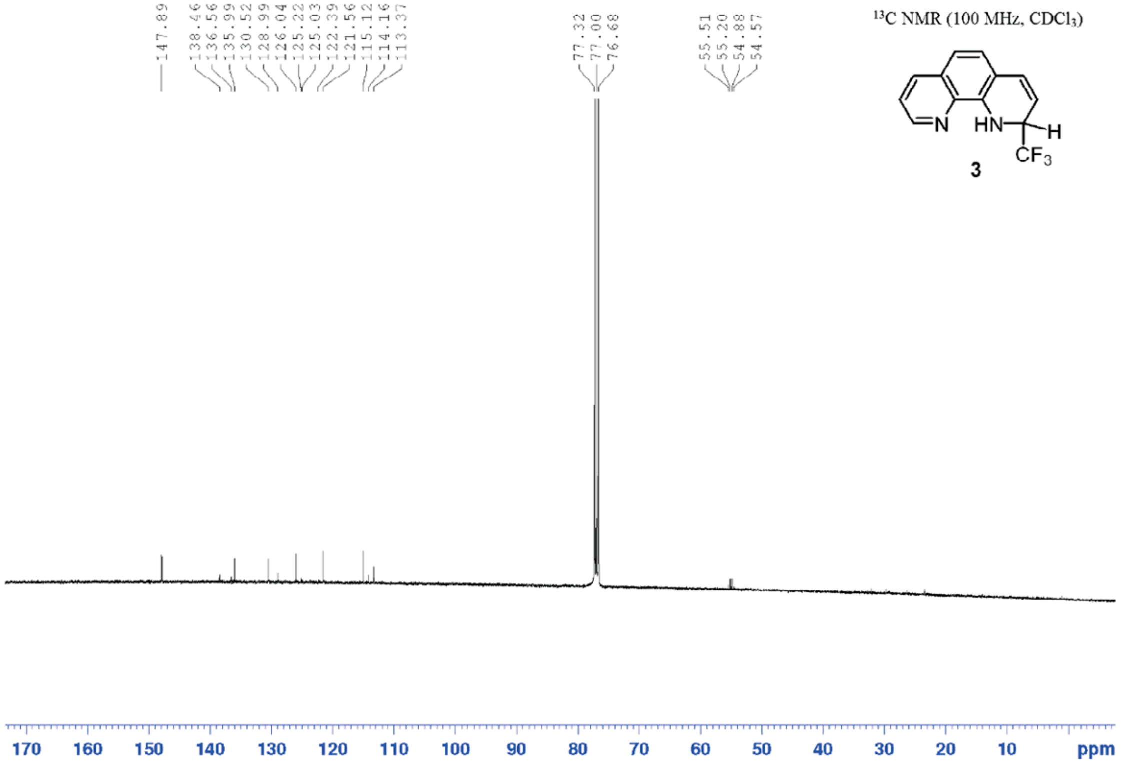

151.06
147.92
147.57
147.22
145.72
145.56
137.83
136.09
129.76
129.10
128.79
125.70
123.59
122.96
120.23
119.00
118.98
77.32
77.00
76.68
^{13}C NMR (100 MHz, CDCl$_3$)
H$_d$
H$_e$
H$_c$
H$_f$
H$_b$
H$_g$
H$_a$
N
N
CF$_3$
2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-66.47
^{19}F NMR (377 MHz, CDCl$_3$)
H$_d$
H$_e$
H$_c$
H$_f$
H$_b$
H$_g$
H$_a$
N
N
CF$_3$
2
0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 ppm



^{1}H NMR (400 MHz, $CDCl_3$)

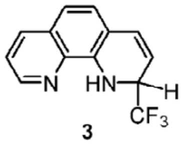
3



^{13}C NMR (100 MHz, $CDCl_3$)

3

^{19}F NMR (377 MHz, $CDCl_3$)



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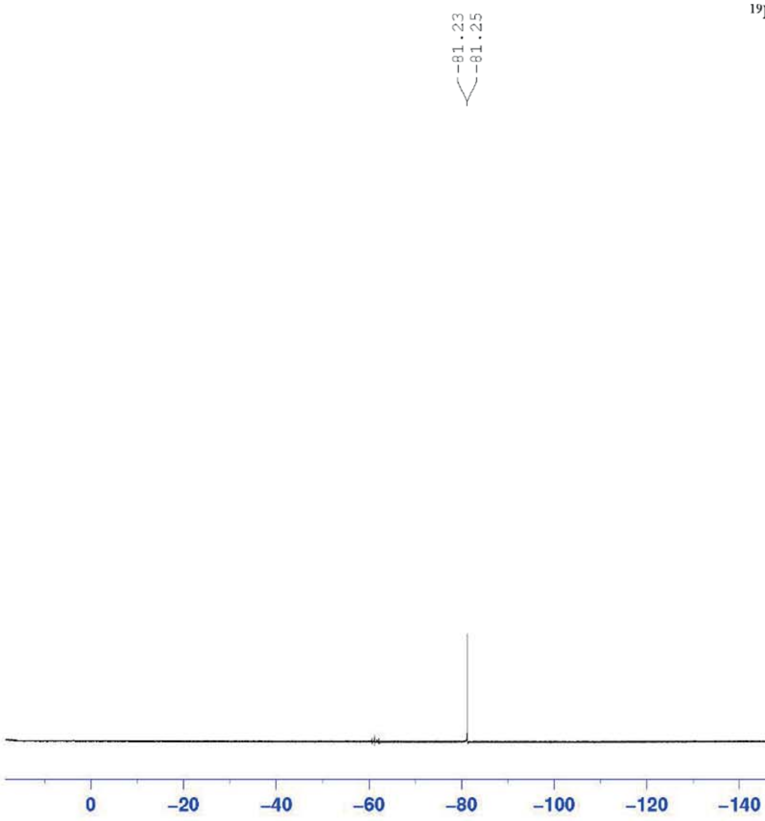
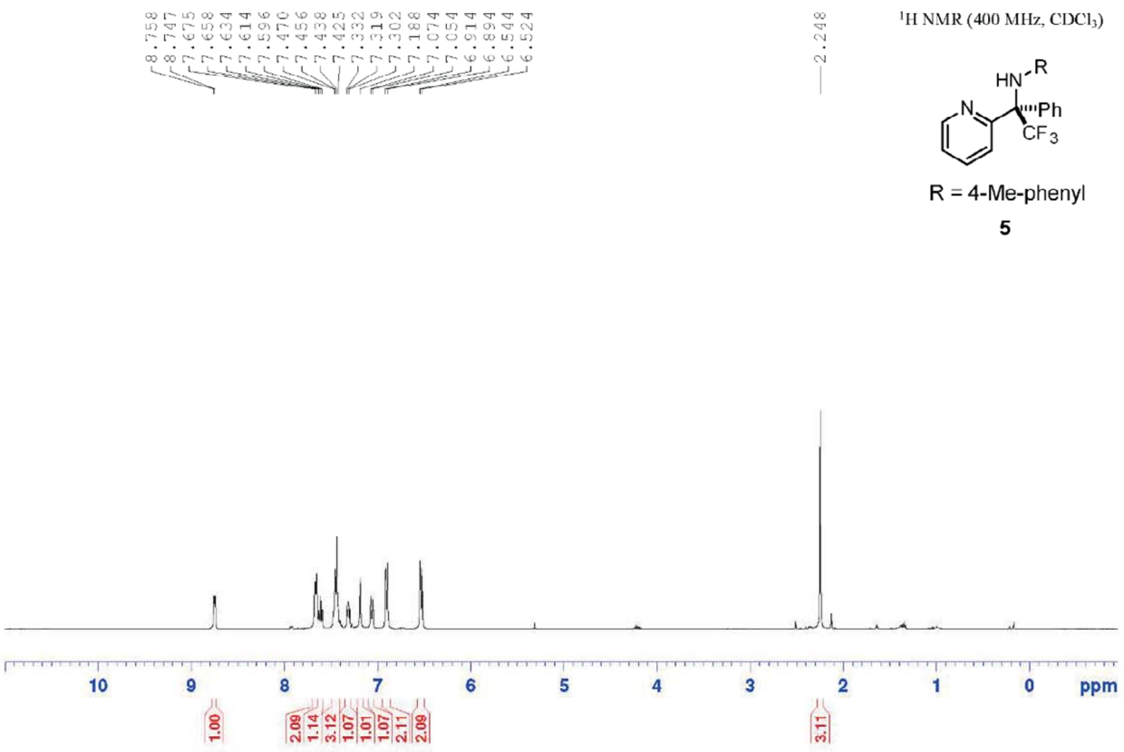
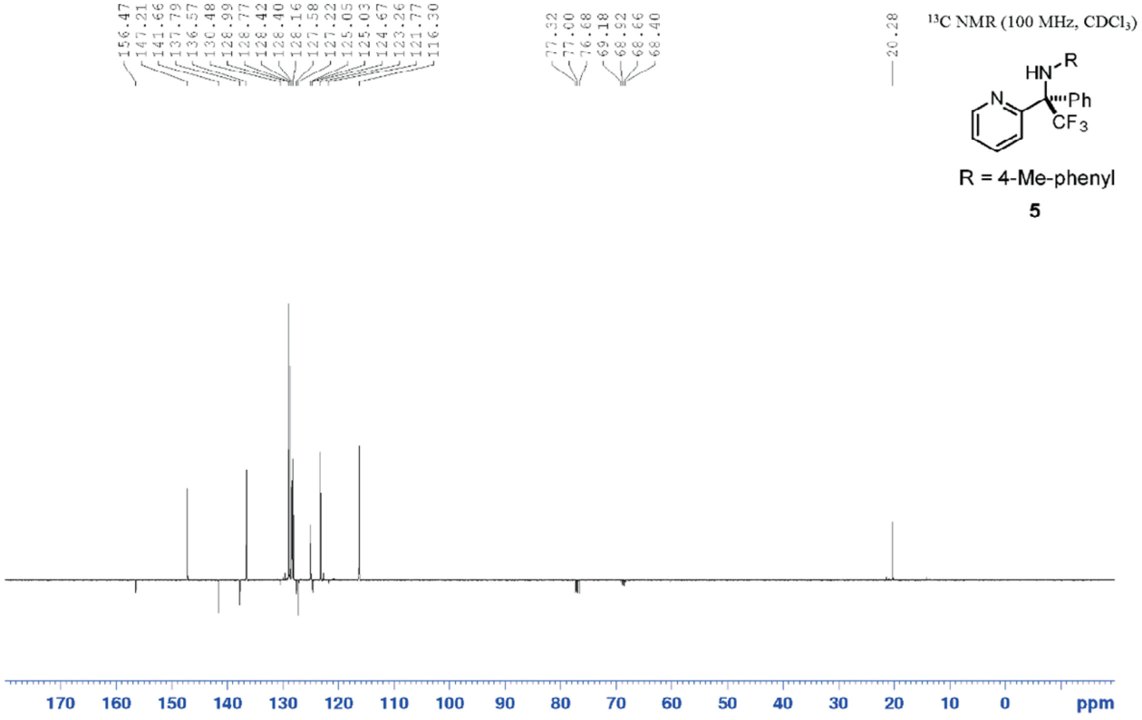




^{1}H NMR (400 MHz, CDCl$_3$)

R = 4-Me-phenyl

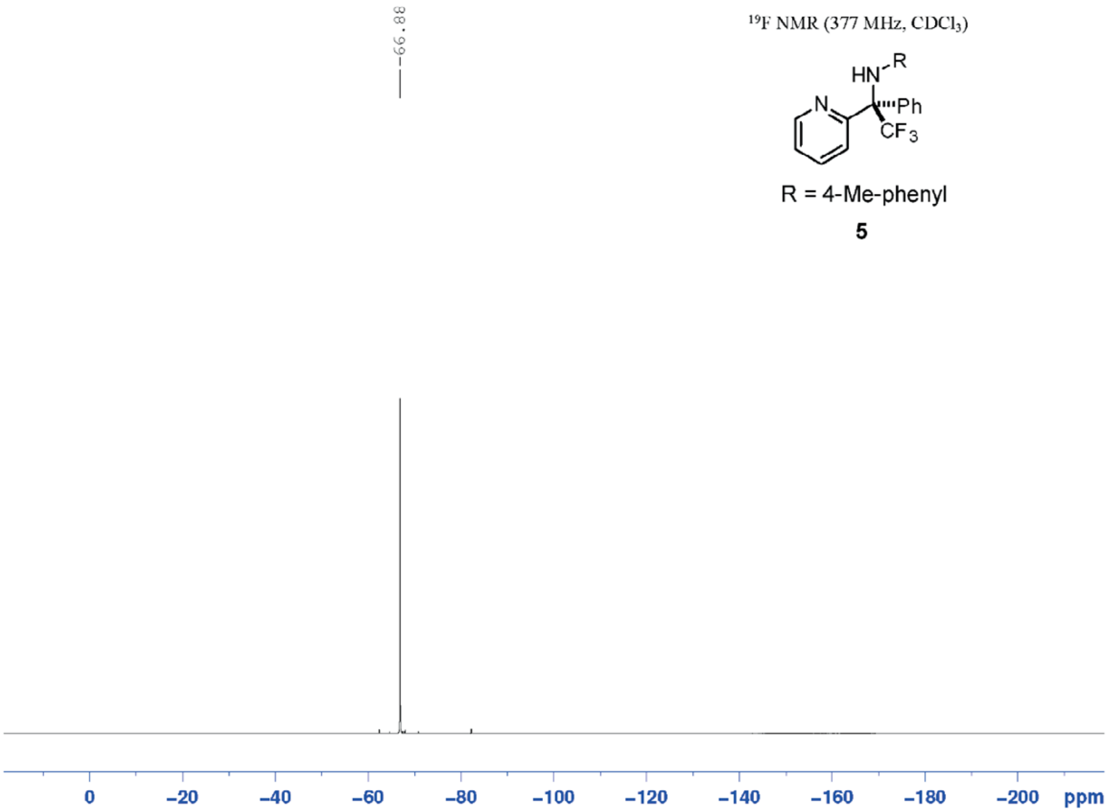
5



^{13}C NMR (100 MHz, CDCl$_3$)

R = 4-Me-phenyl

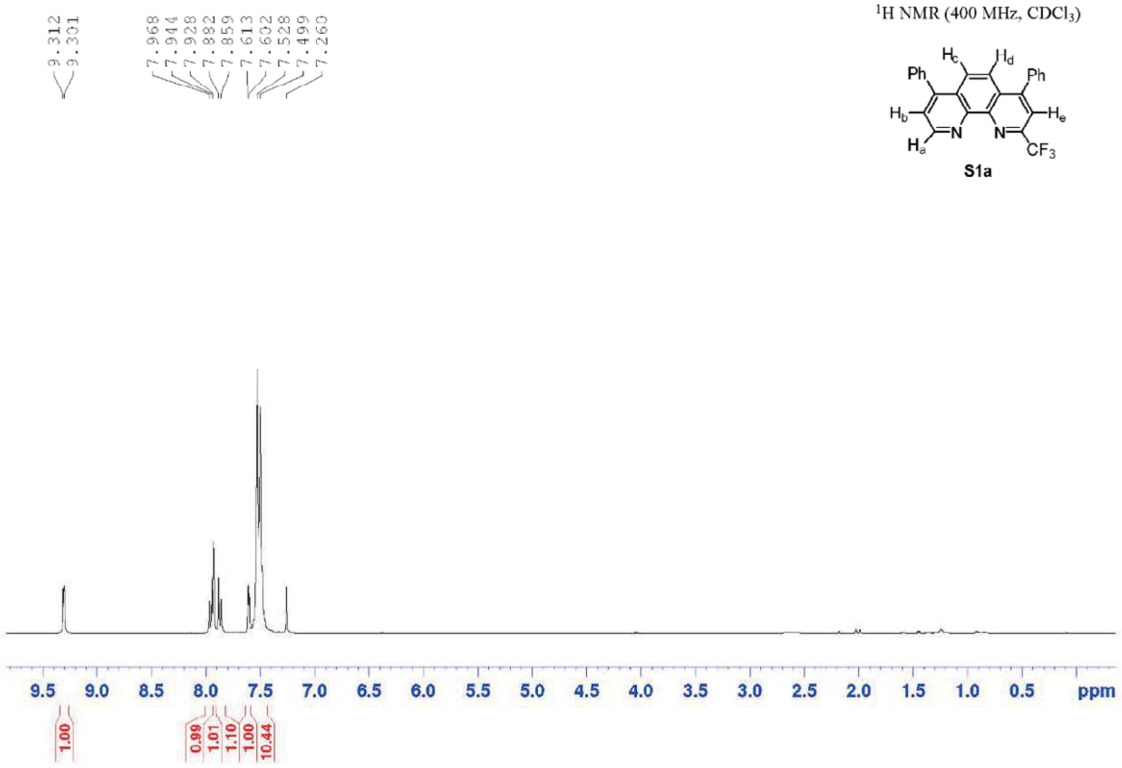
5



^{19}F NMR (377 MHz, $CDCl_3$)

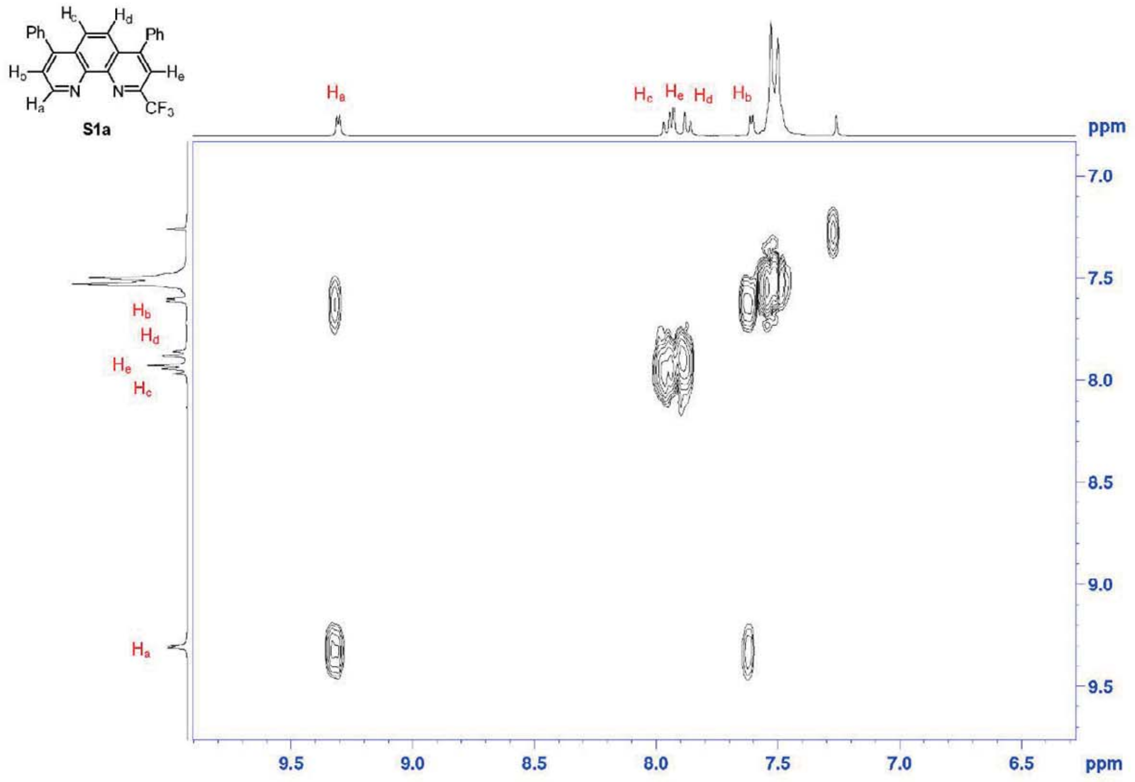
R = 4-Me-phenyl

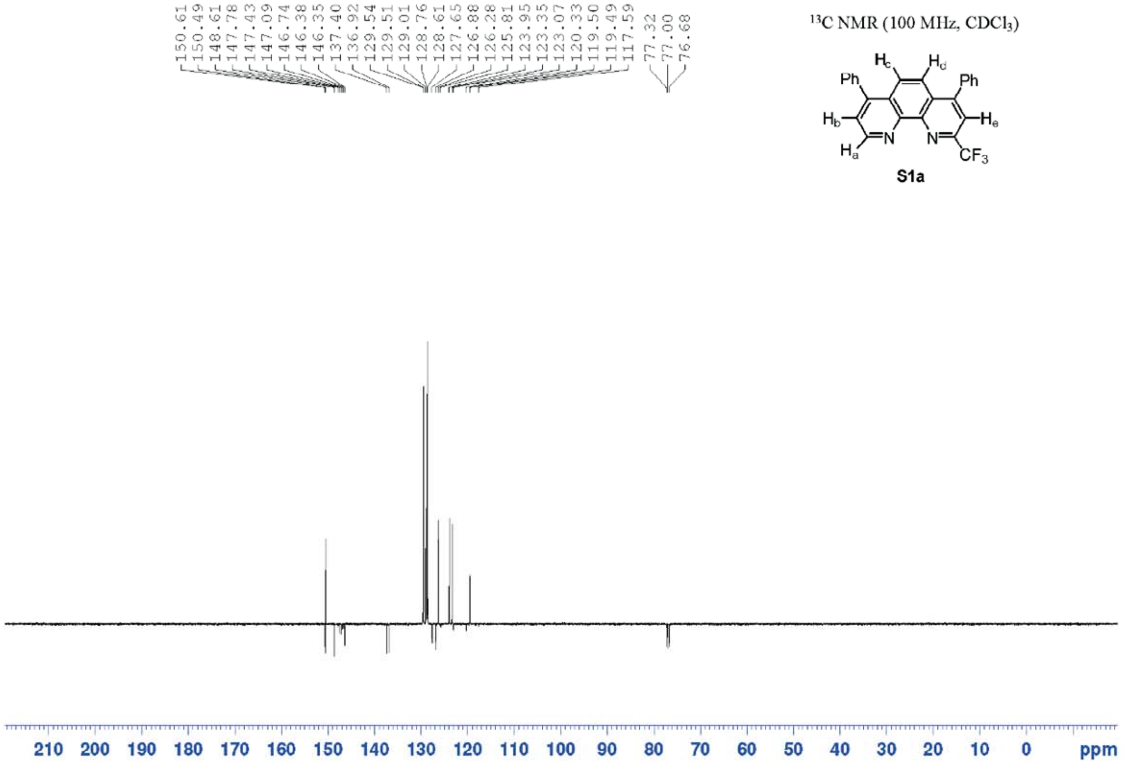
5



^1H NMR (400 MHz, $CDCl_3$)

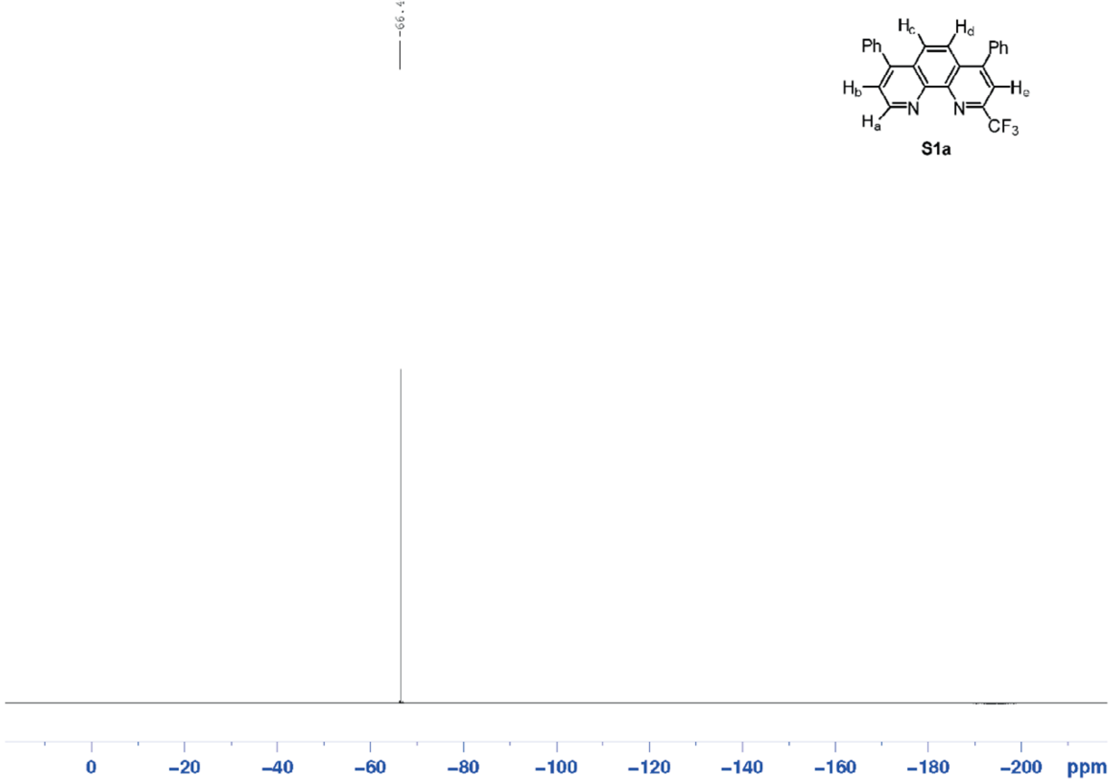
COSY





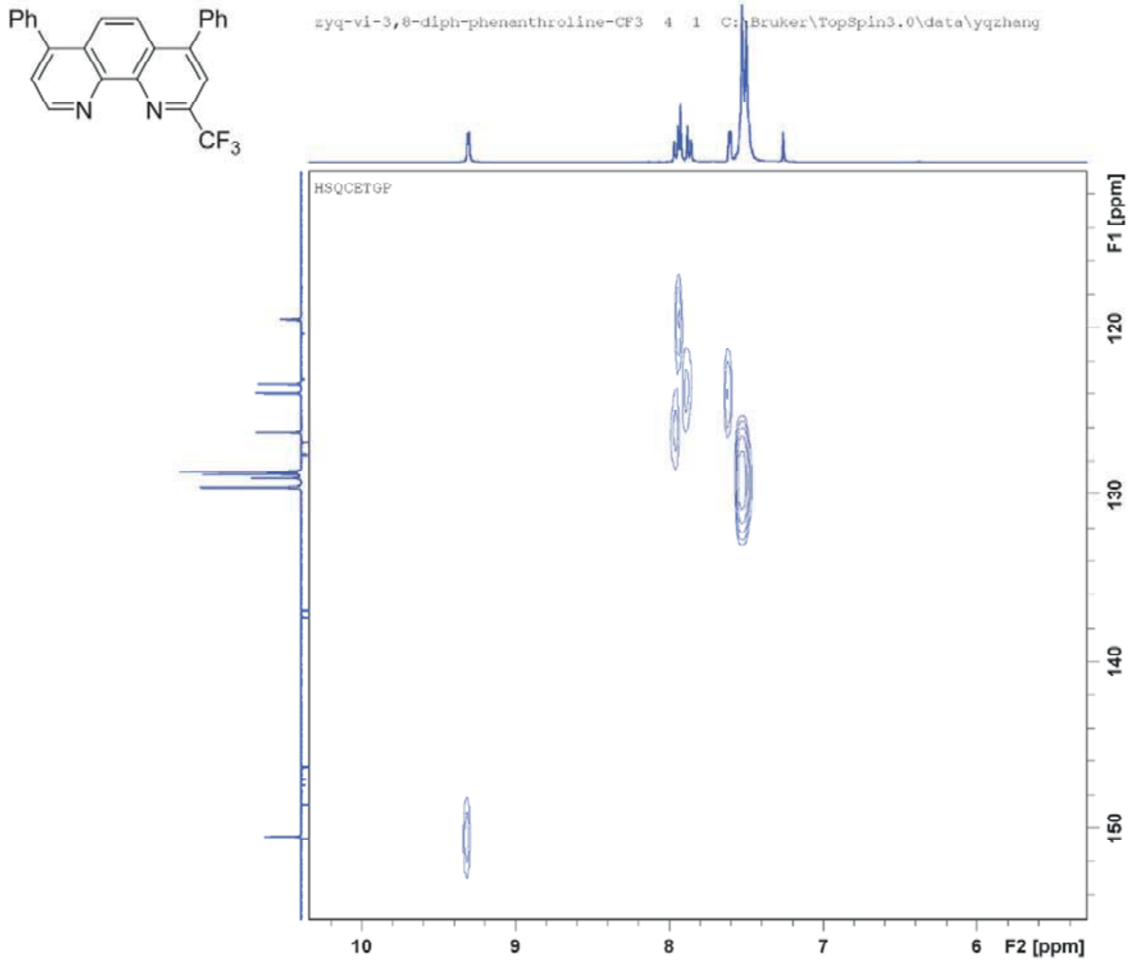
^{13}C NMR (100 MHz, CDCl$_3$)

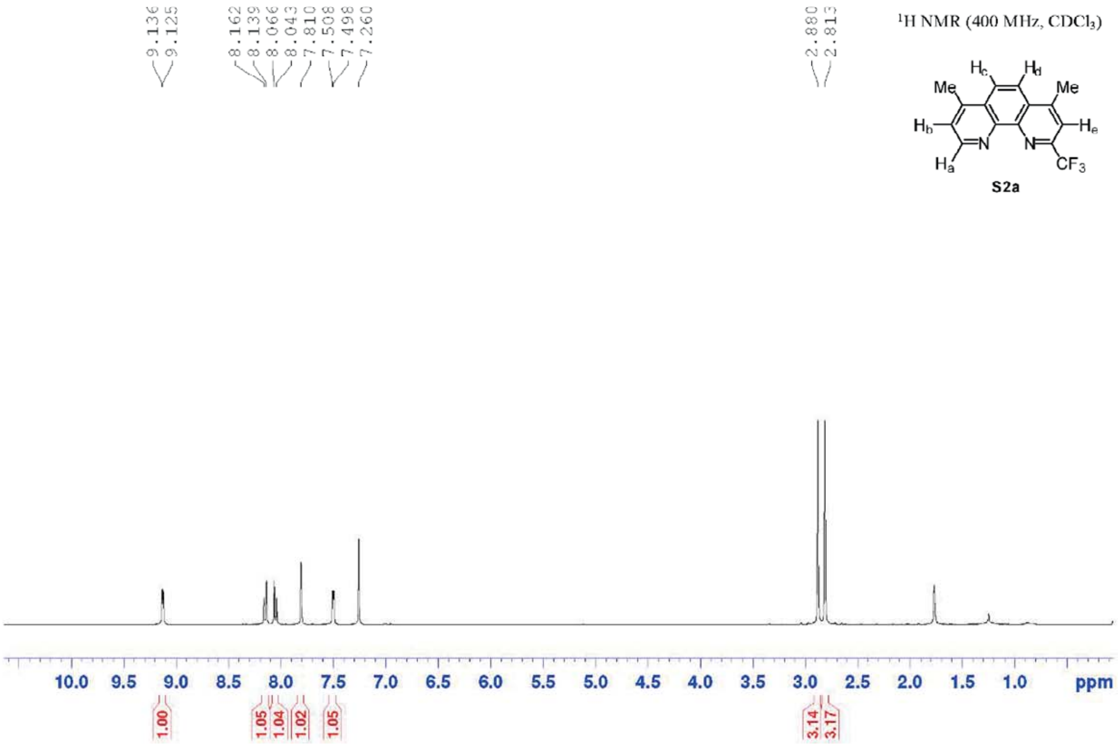
S1a

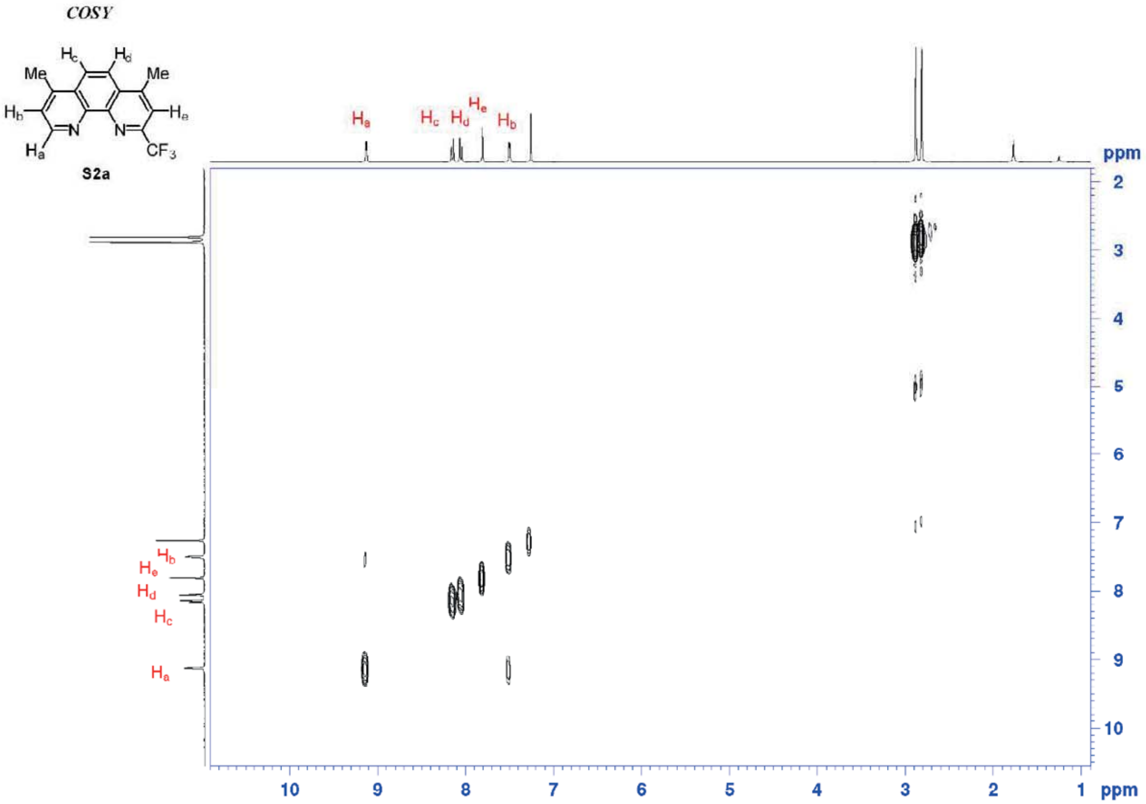


^{19}F NMR (377 MHz, CDCl$_3$)

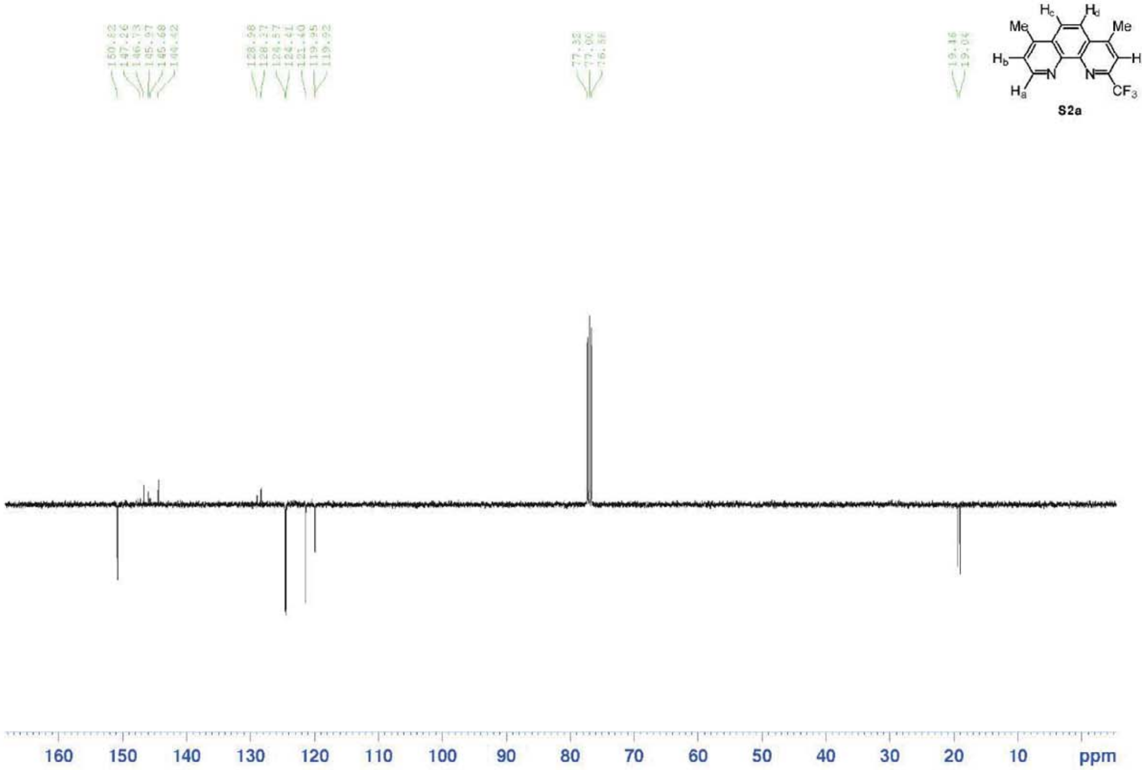
S1a


Ph
Ph
N
N
CF3
zyq-vi-3,8-diph-phenanthroline-CF3 4 1 C:\Bruker\TopSpin3.0\data\yqzhang
HSQCETGP
F1 [ppm]
120
130
140
150
10
9
8
7
6
F2 [ppm]

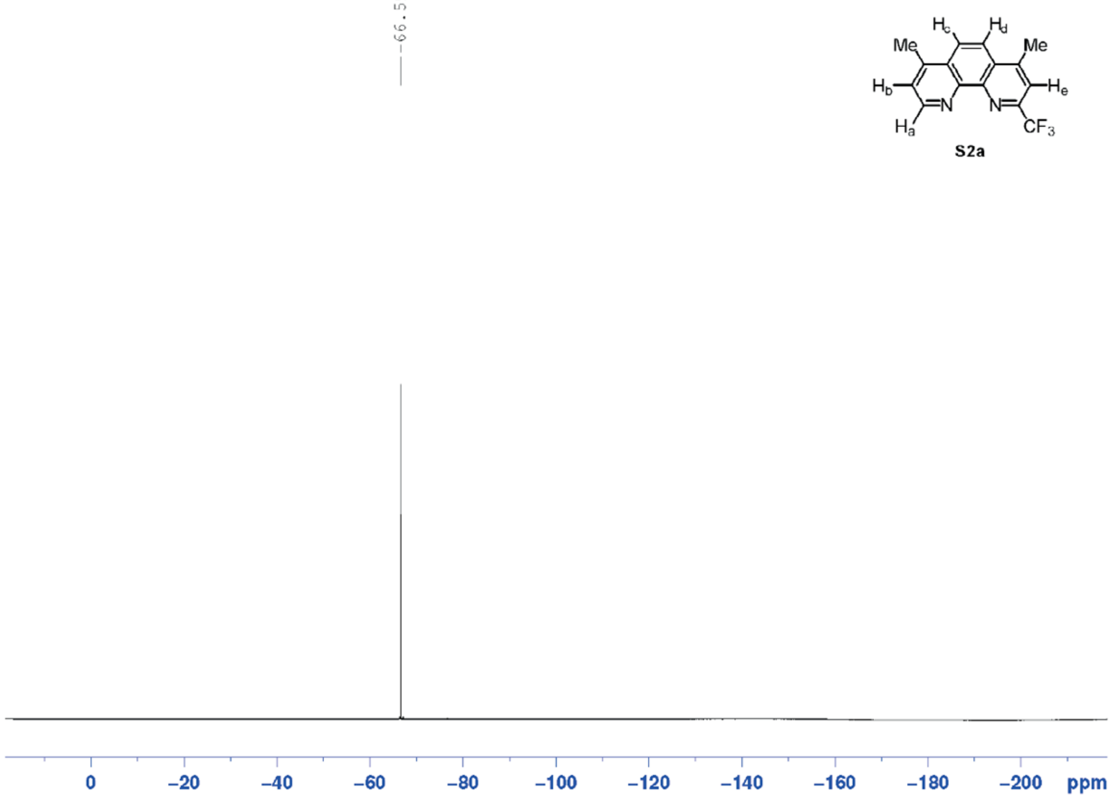

9.136
9.125
8.162
8.139
8.066
8.043
7.810
7.508
7.498
7.260
2.880
2.813
¹H NMR (400 MHz, CDCl₃)
Hc
Hd
Me
Me
Hb
He
N
N
Ha
CF3
S2a
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.05
1.04
1.02
1.05
3.14
3.17

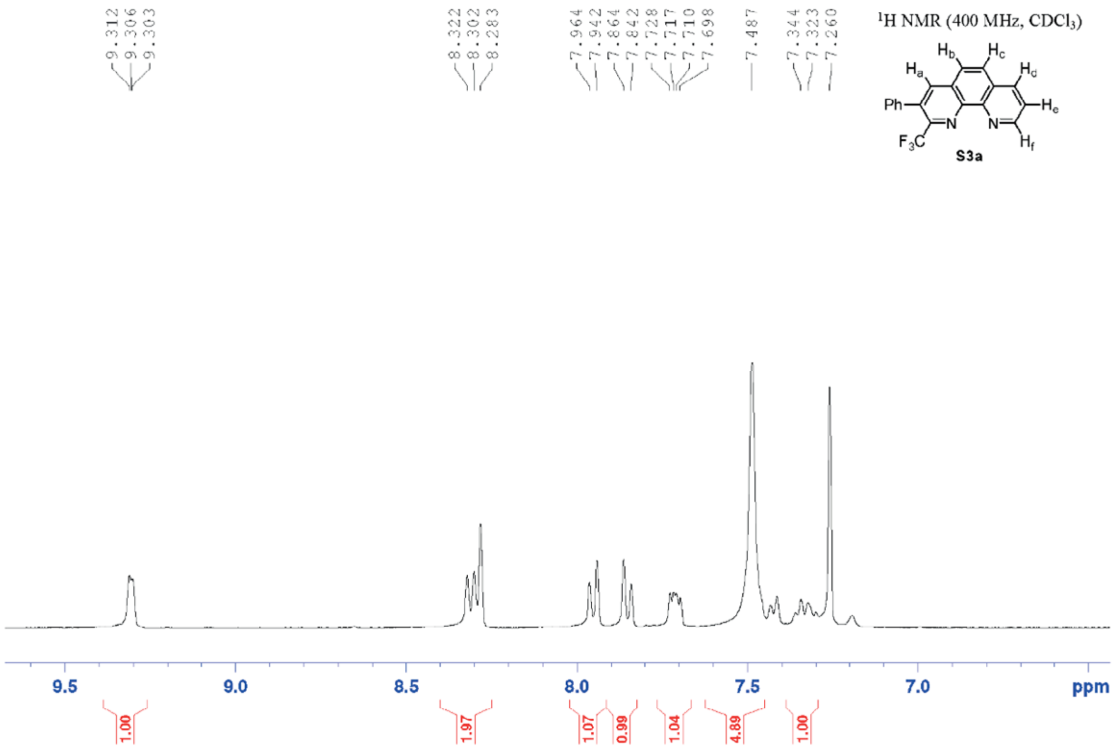

COSY
Hc
Hd
Me
Me
Hb
He
N
N
Ha
CF3
S2a
Ha
Hc
Hd
He
Hb
ppm
2
3
4
5
6
7
8
9
10
Hb
He
Hd
Hc
Ha
10
9
8
7
6
5
4
3
2
1
ppm

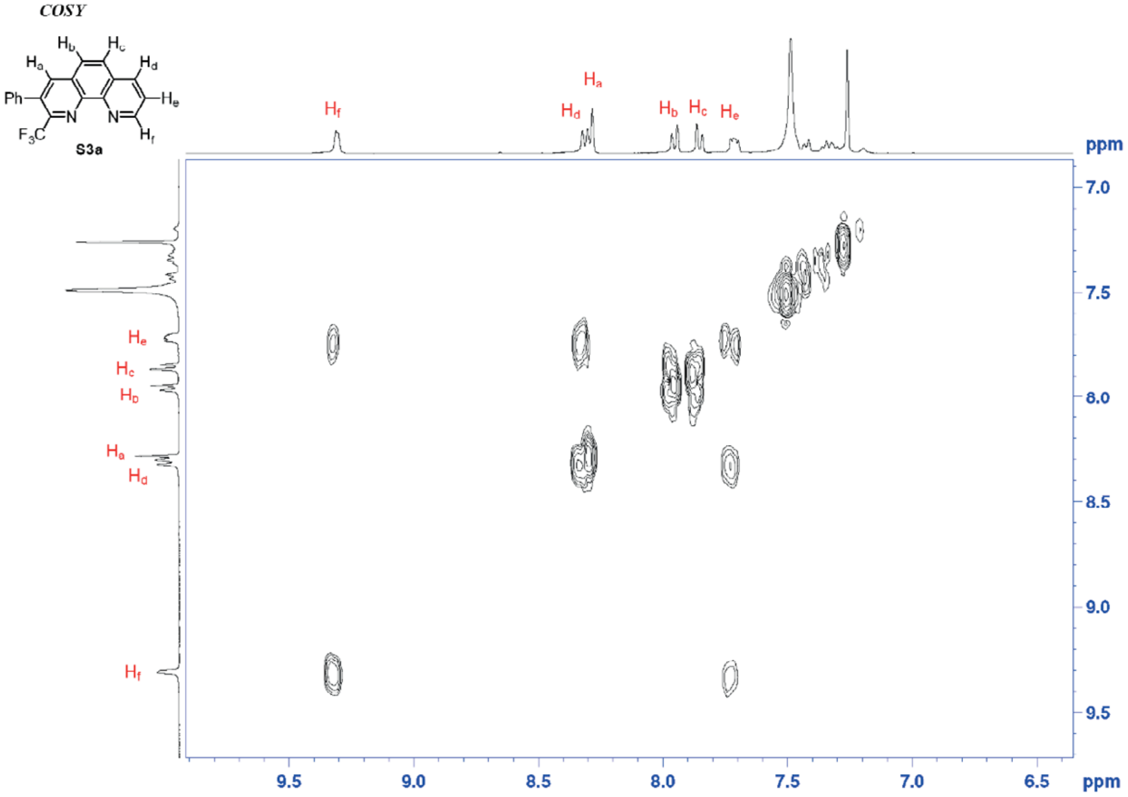
^{13}C NMR (100 MHz, $CDCl_3$)

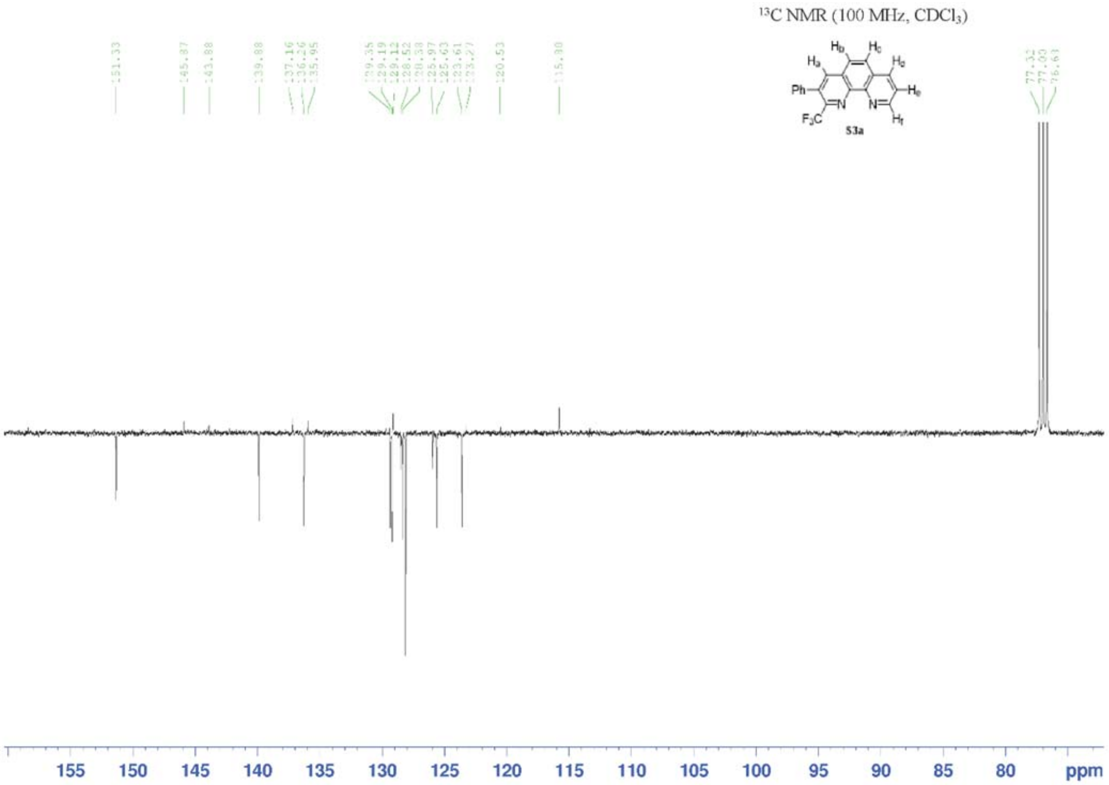


^{19}F NMR (377 MHz, $CDCl_3$)

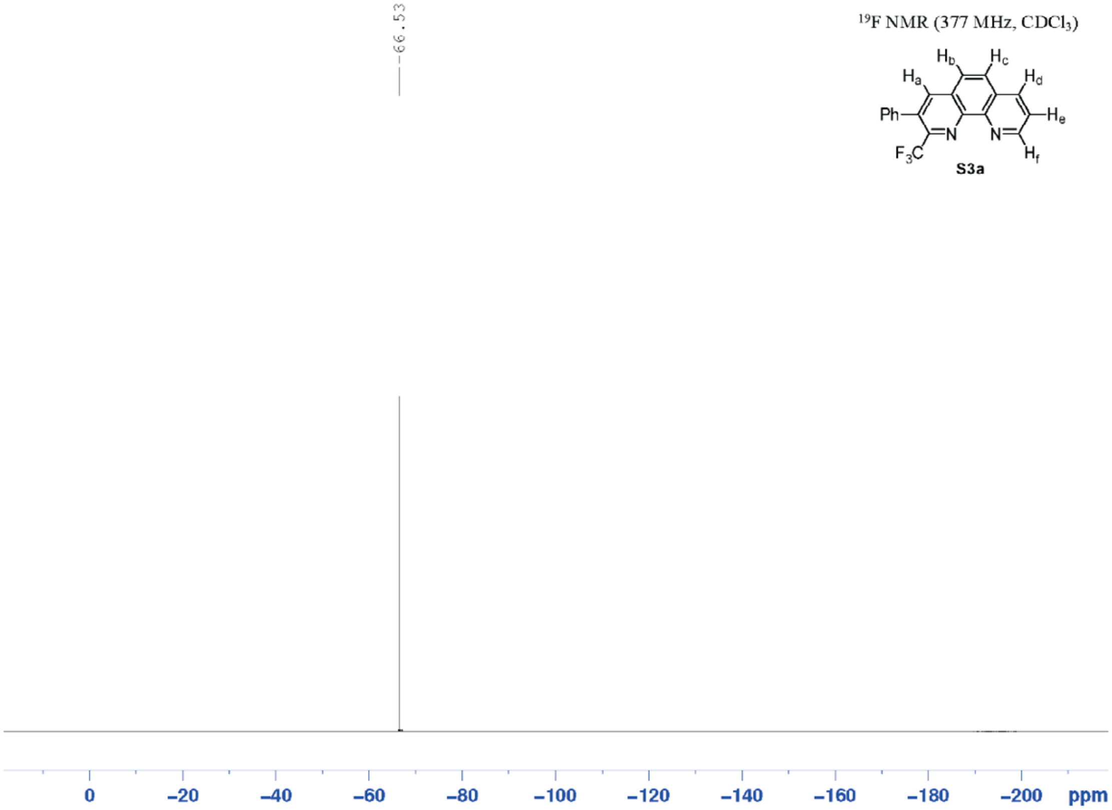



^{1}H NMR (400 MHz, CDCl$_3$)
S3a
Ph
F$_3$C
N
N
H$_a$
H$_b$
H$_c$
H$_d$
H$_e$
H$_f$
9.312
9.306
9.303
8.322
8.302
8.283
7.964
7.942
7.864
7.842
7.728
7.717
7.710
7.698
7.487
7.344
7.323
7.260
9.5
9.0
8.5
8.0
7.5
7.0
ppm
1.00
1.97
1.07
0.99
1.04
4.89
1.00

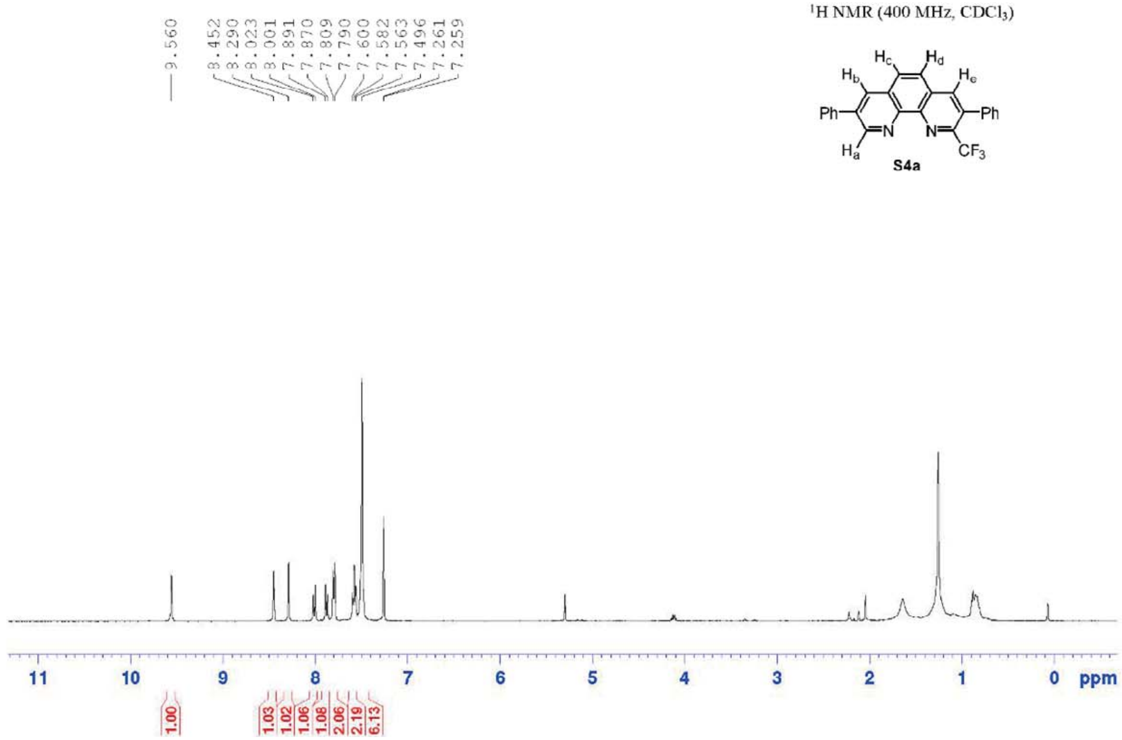

COSY
S3a
Ph
F$_3$C
N
N
H$_a$
H$_b$
H$_c$
H$_d$
H$_e$
H$_f$
H$_f$
H$_d$
H$_a$
H$_b$
H$_c$
H$_e$
ppm
H$_e$
H$_c$
H$_b$
H$_a$
H$_d$
H$_f$
7.0
7.5
8.0
8.5
9.0
9.5
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm



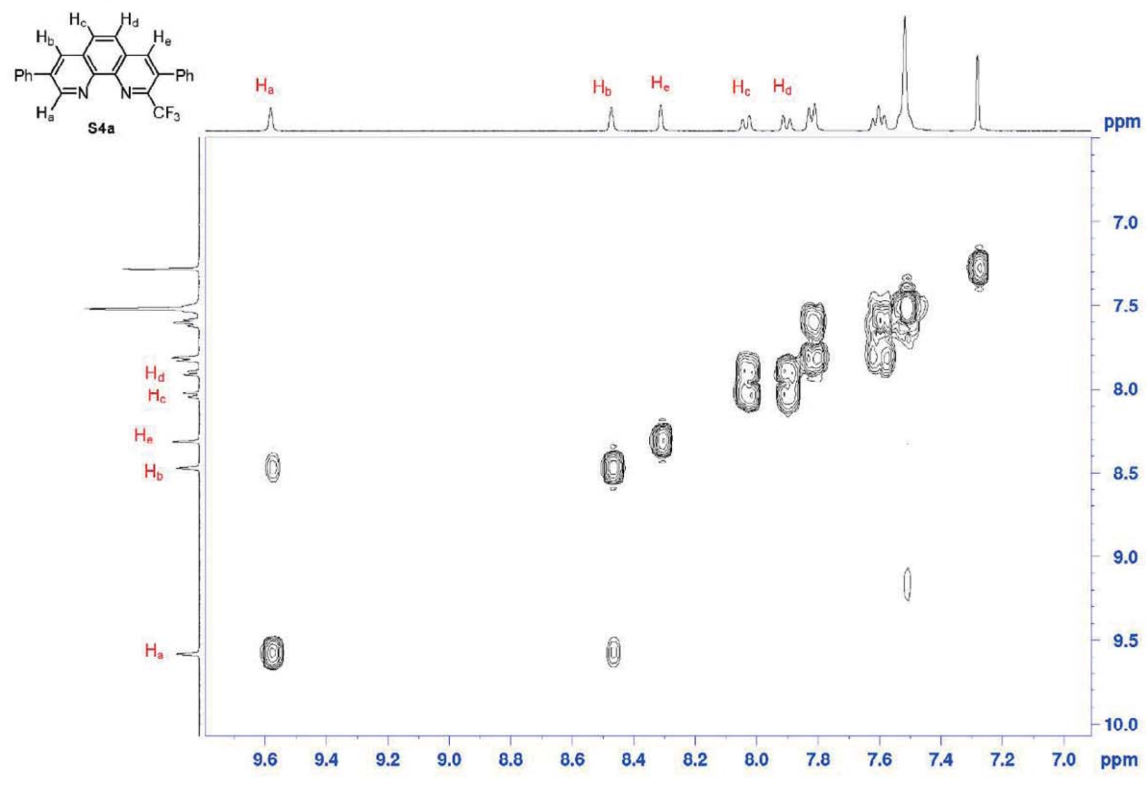
^{13}C NMR (100 MHz, $CDCl_3$)

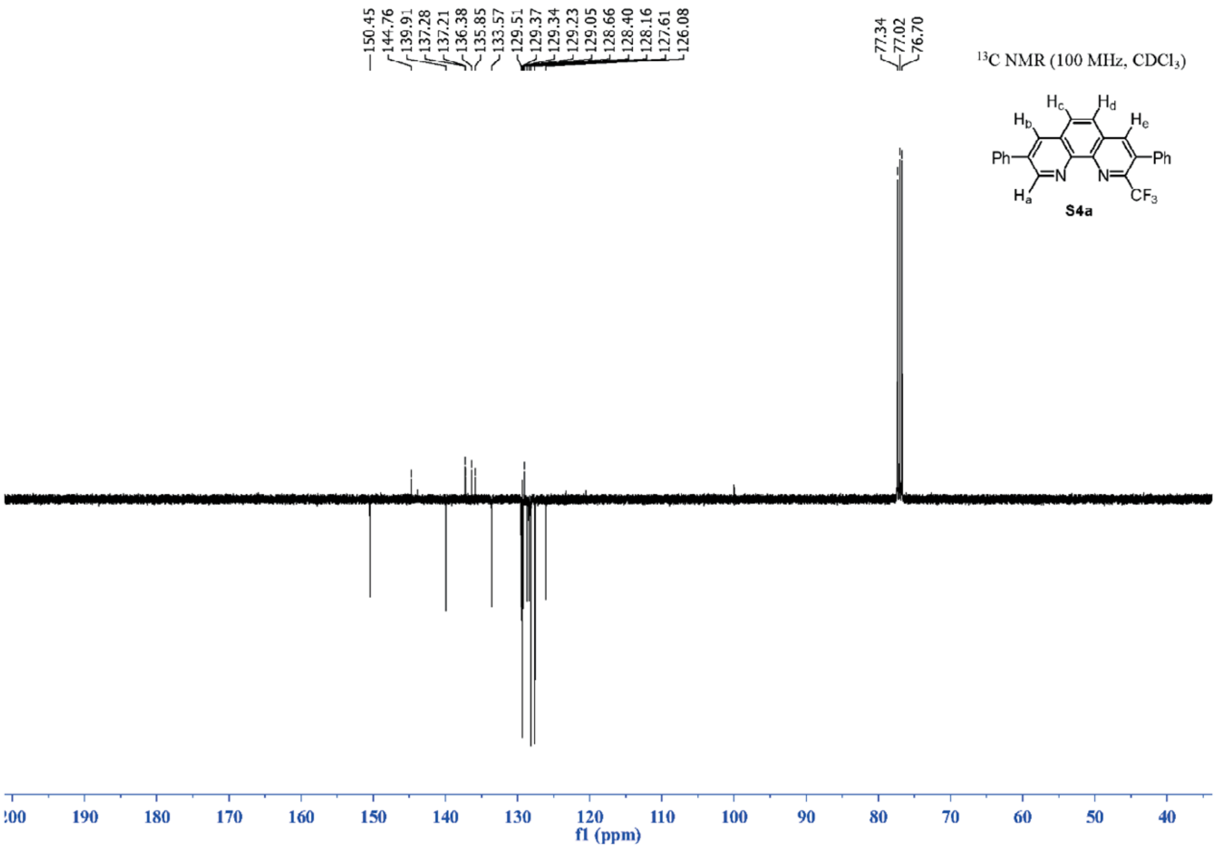


^{19}F NMR (377 MHz, $CDCl_3$)


9.560
8.452
8.290
8.023
8.001
7.891
7.870
7.809
7.790
7.600
7.582
7.563
7.496
7.261
7.259
¹H NMR (400 MHz, CDCl₃)
Hc
Hd
Hb
He
Ph
Ph
N
N
Ha
CF₃
S4a
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
1.02
1.06
1.08
2.06
2.19
6.13

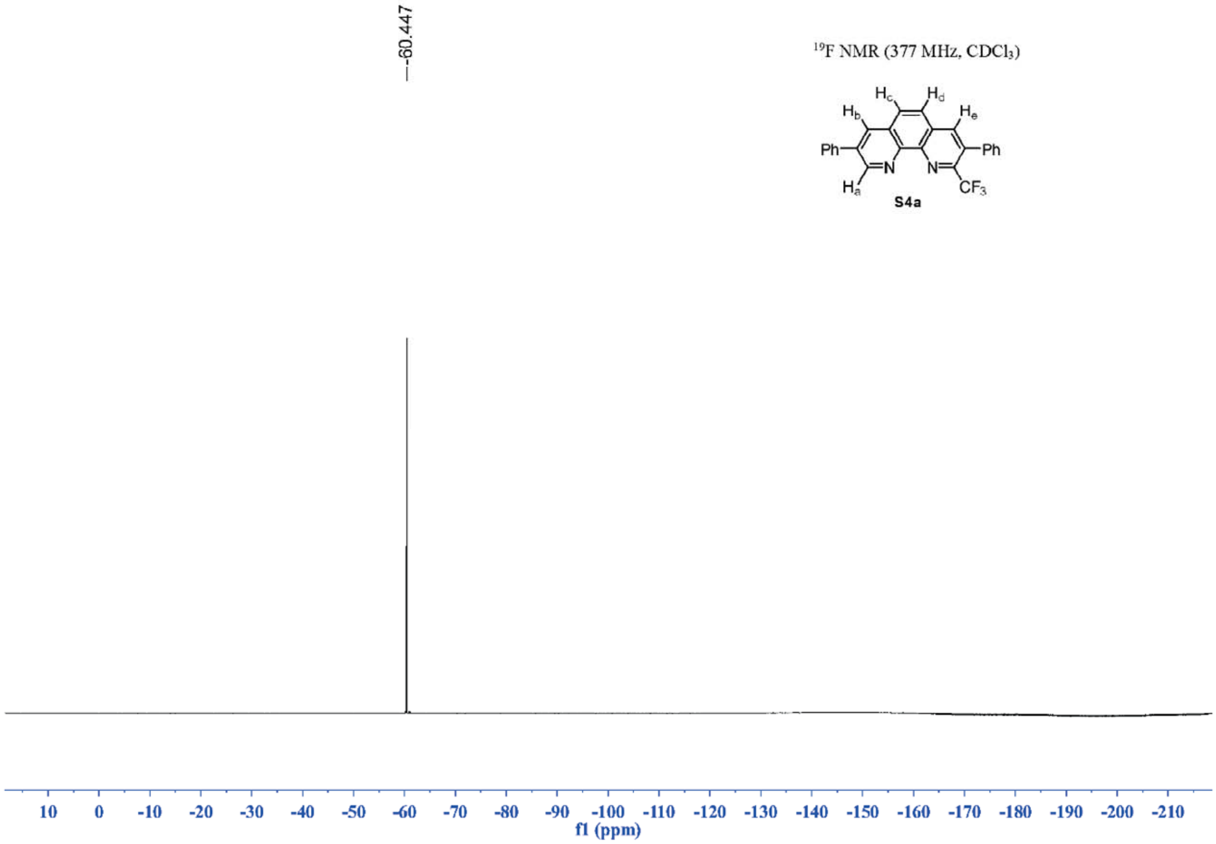
COSY


Hc
Hd
Hb
He
Ph
Ph
N
N
Ha
CF₃
S4a
Ha
Hb
He
Hc
Hd
ppm
Hd
Hc
He
Hb
Ha
7.0
7.5
8.0
8.5
9.0
9.5
10.0
ppm
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
ppm



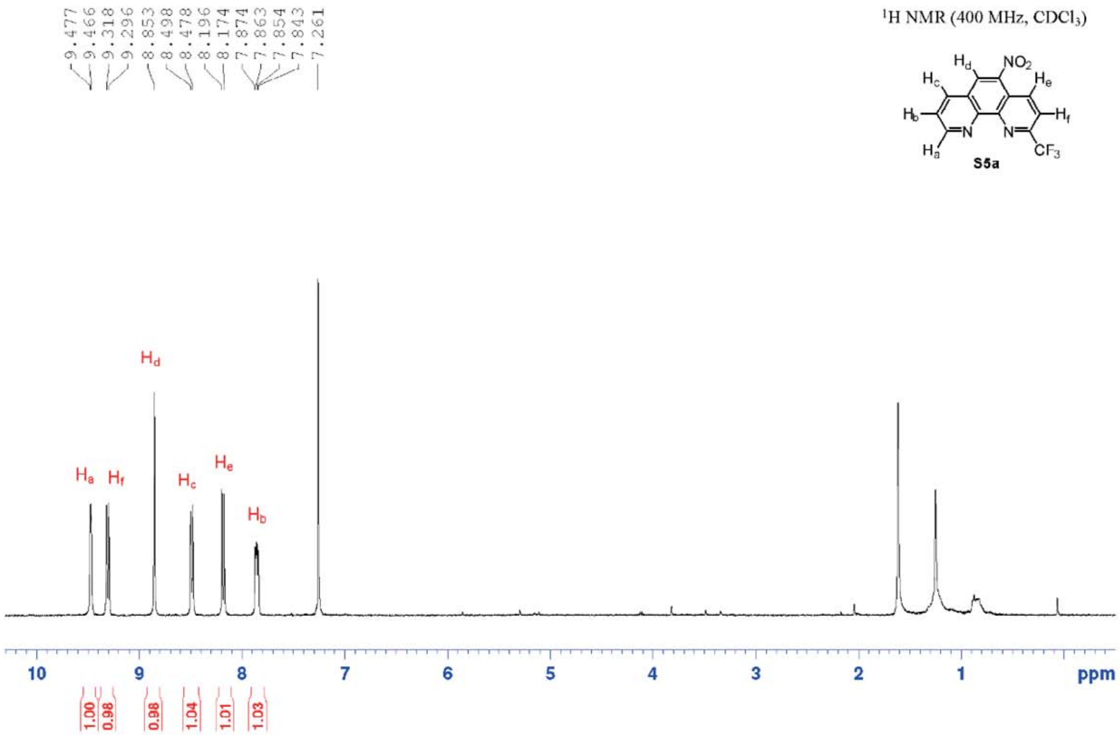
^{13}C NMR (100 MHz, $CDCl_3$)

S4a

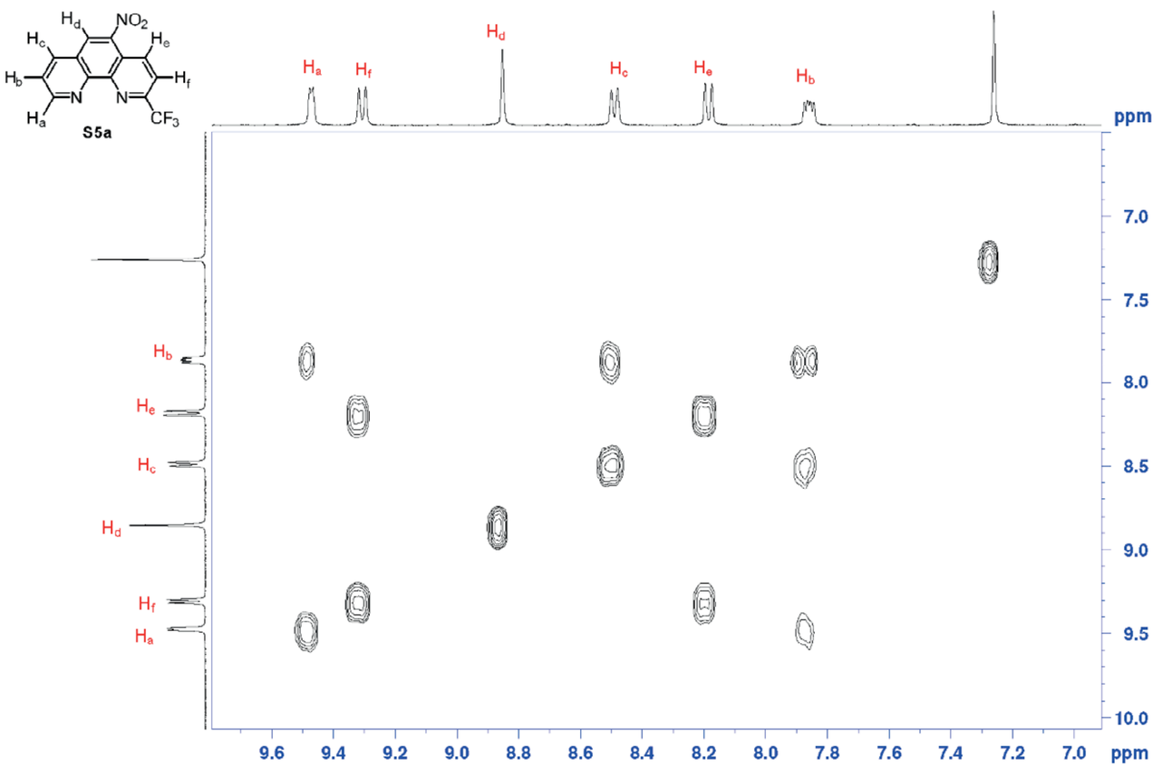


^{19}F NMR (377 MHz, $CDCl_3$)

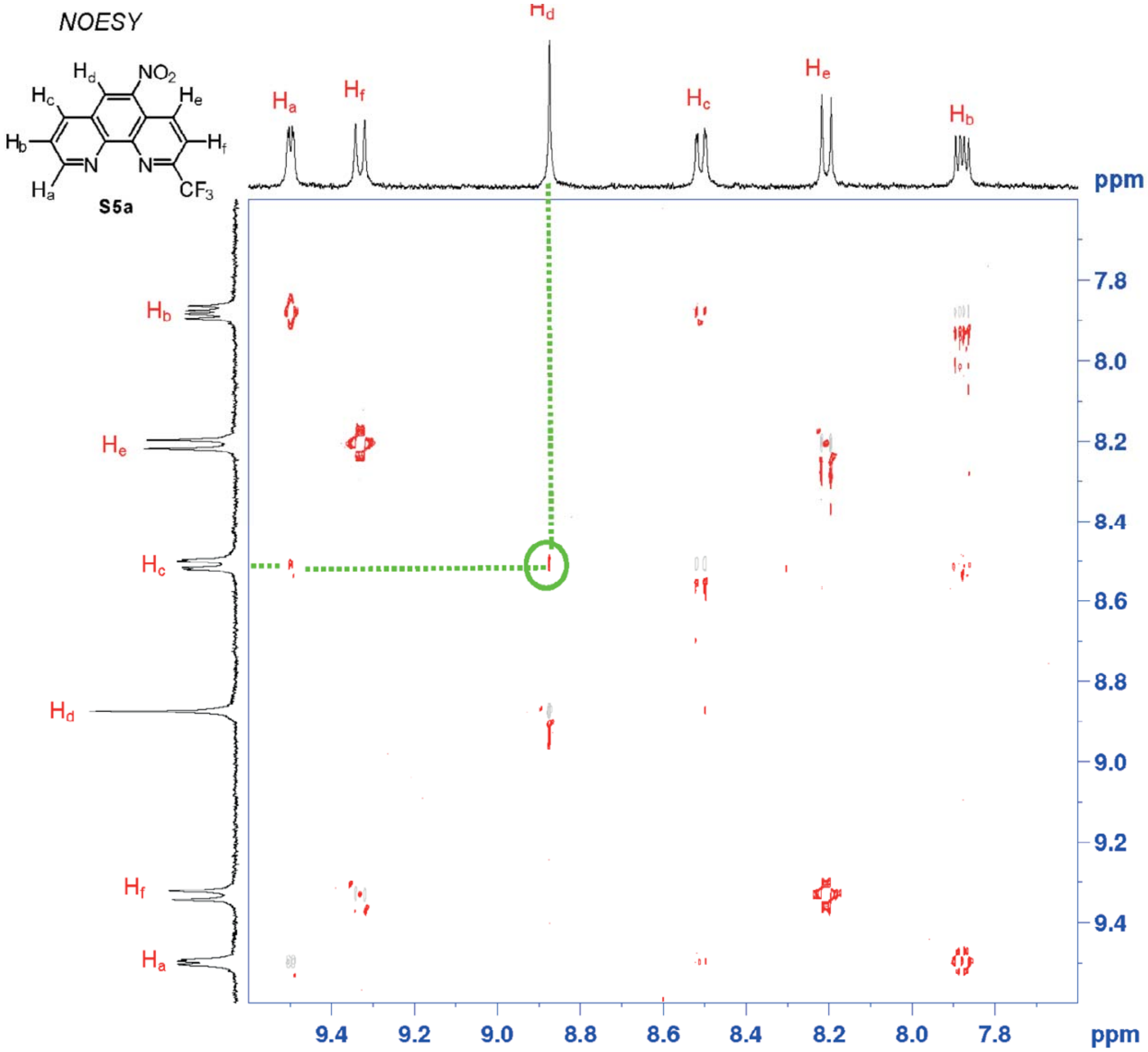
S4a

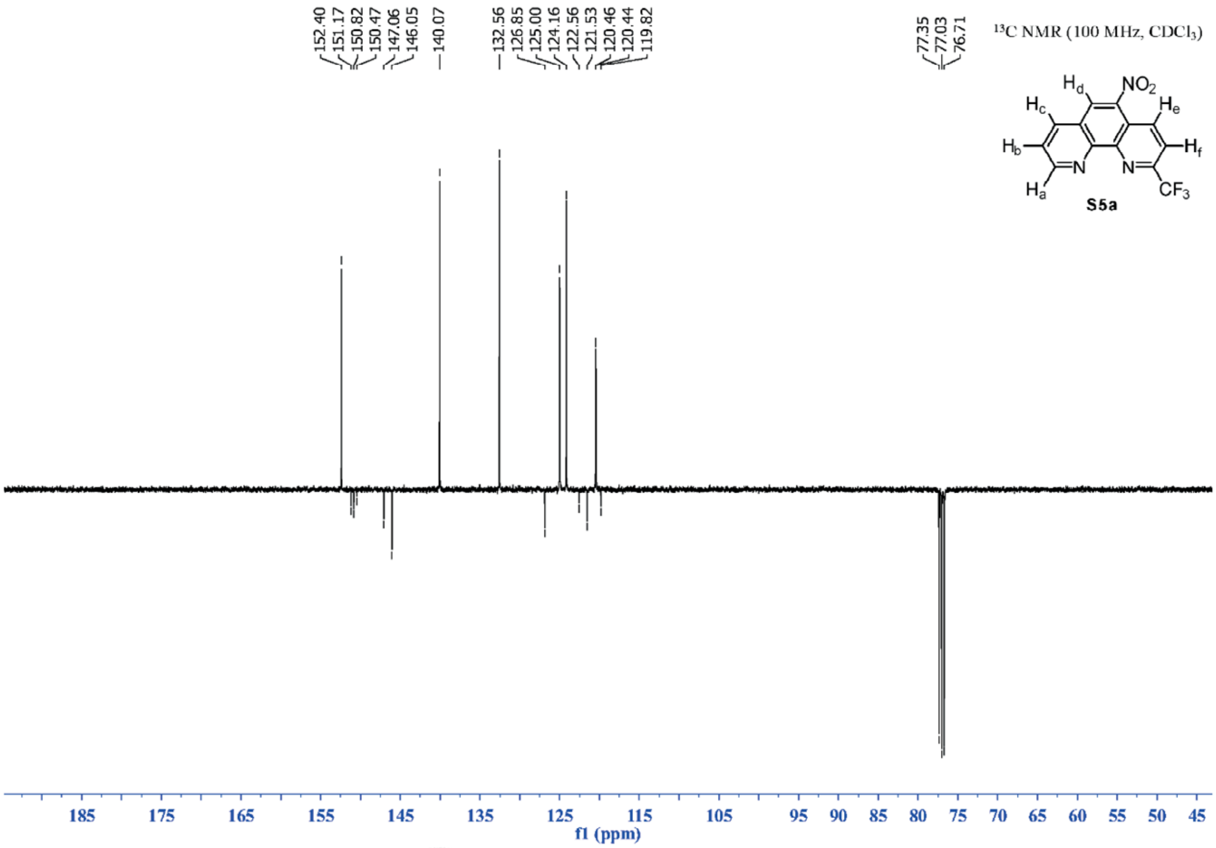


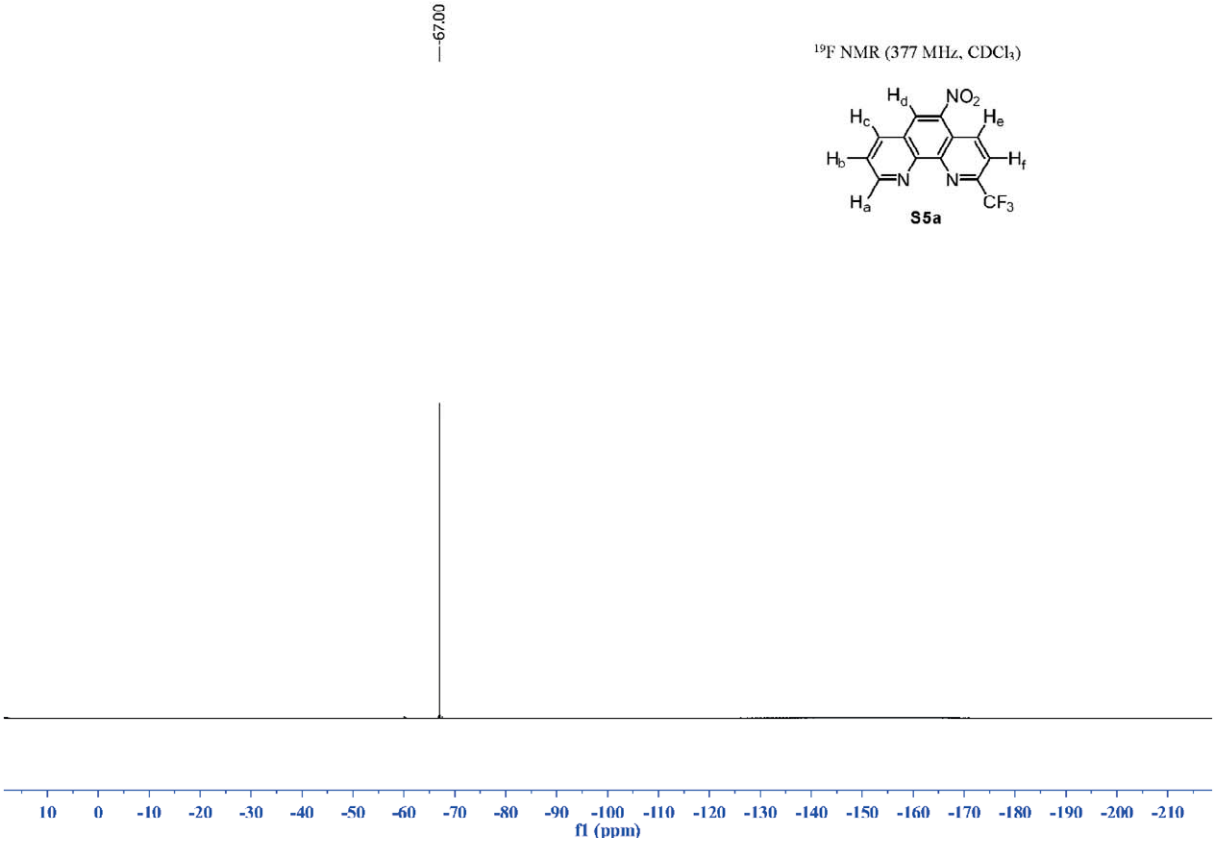
^{1}H NMR (400 MHz, CDCl$_3$)

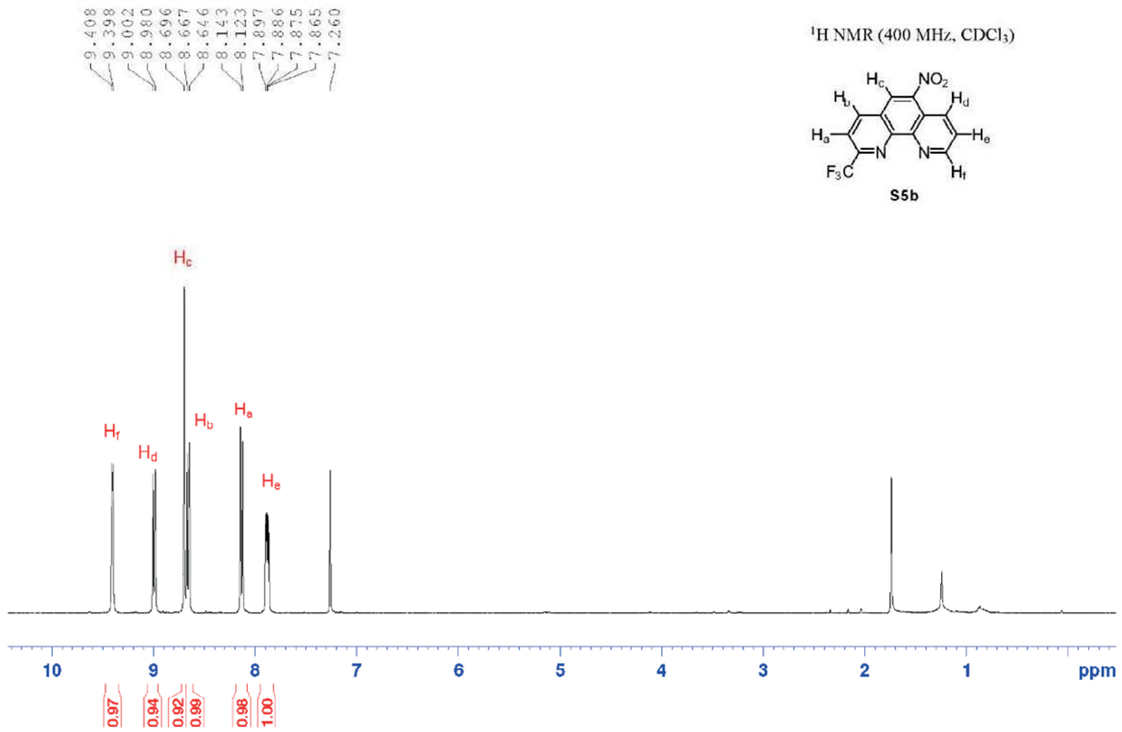


COSY

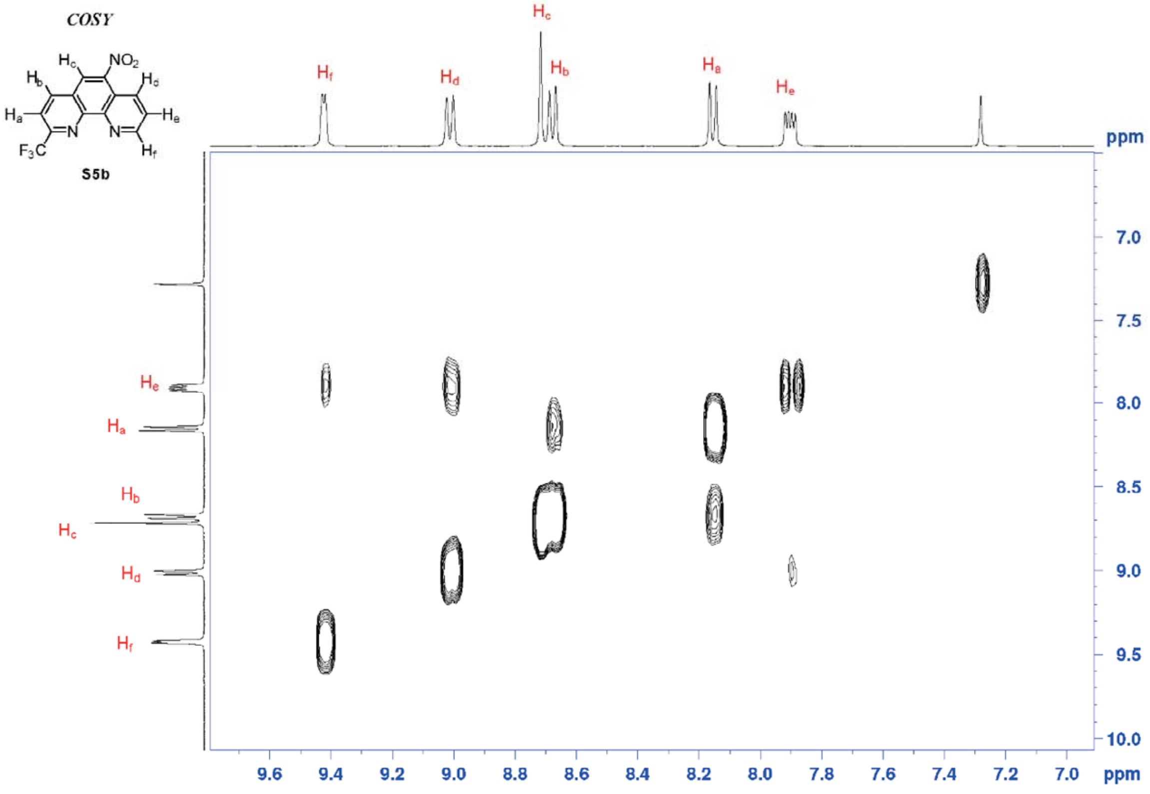

NOESY
H_d
NO2
H_c
H_e
H_b
H_f
N
N
H_a
CF3
S5a
H_a
H_f
H_d
H_c
H_e
H_b
ppm
H_b
H_e
H_c
H_d
H_f
H_a
7.8
8.0
8.2
8.4
8.6
8.8
9.0
9.2
9.4
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
ppm

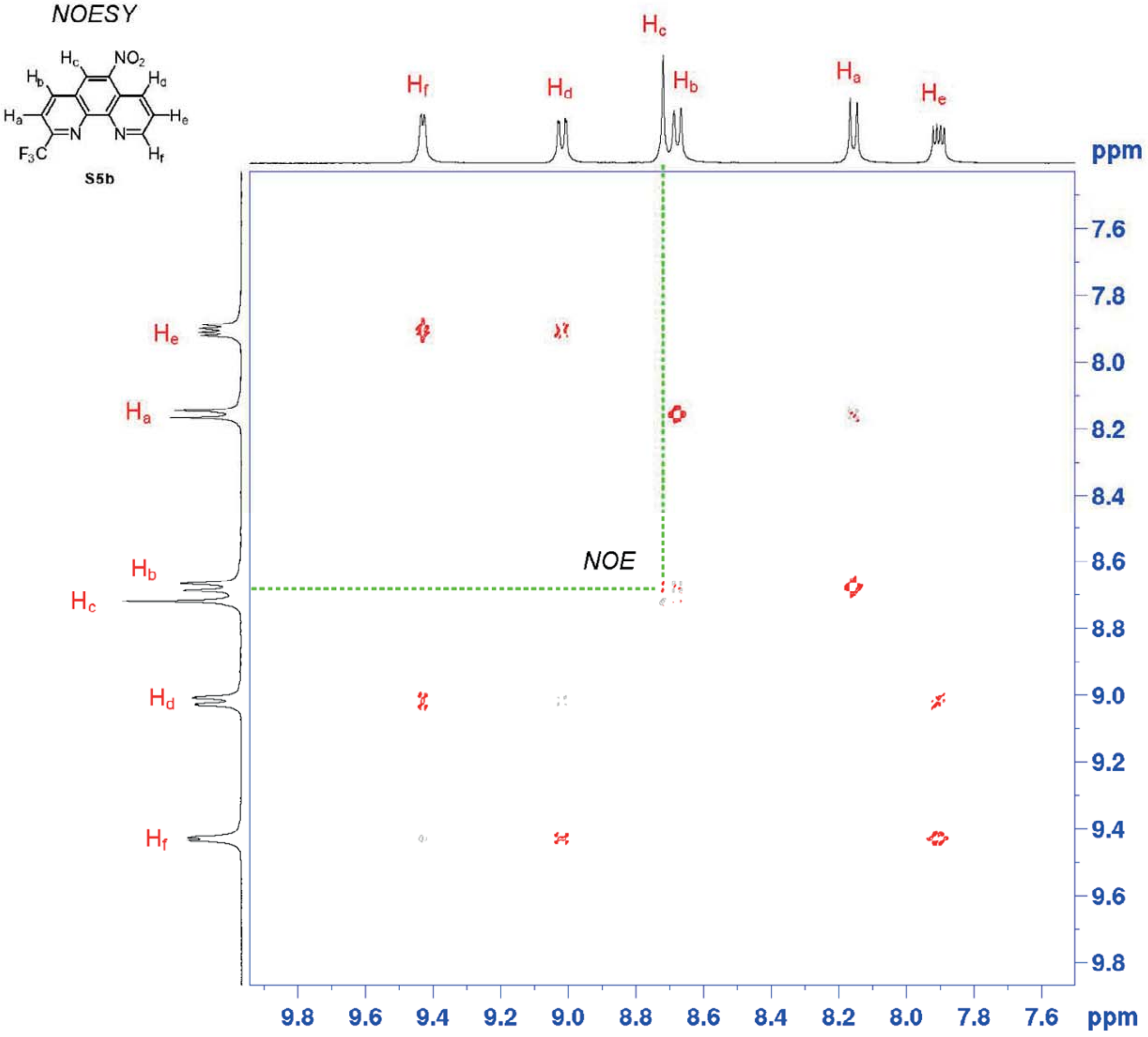

152.40
151.17
150.82
150.47
147.06
146.05
140.07
132.56
126.85
125.00
124.16
122.56
121.53
120.46
120.44
119.82
77.35
77.03
76.71
13C NMR (100 MHz, CDCl3)
Hd
NO2
Hc
He
Hb
Hf
N
N
Ha
CF3
S5a
185
175
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
f1 (ppm)

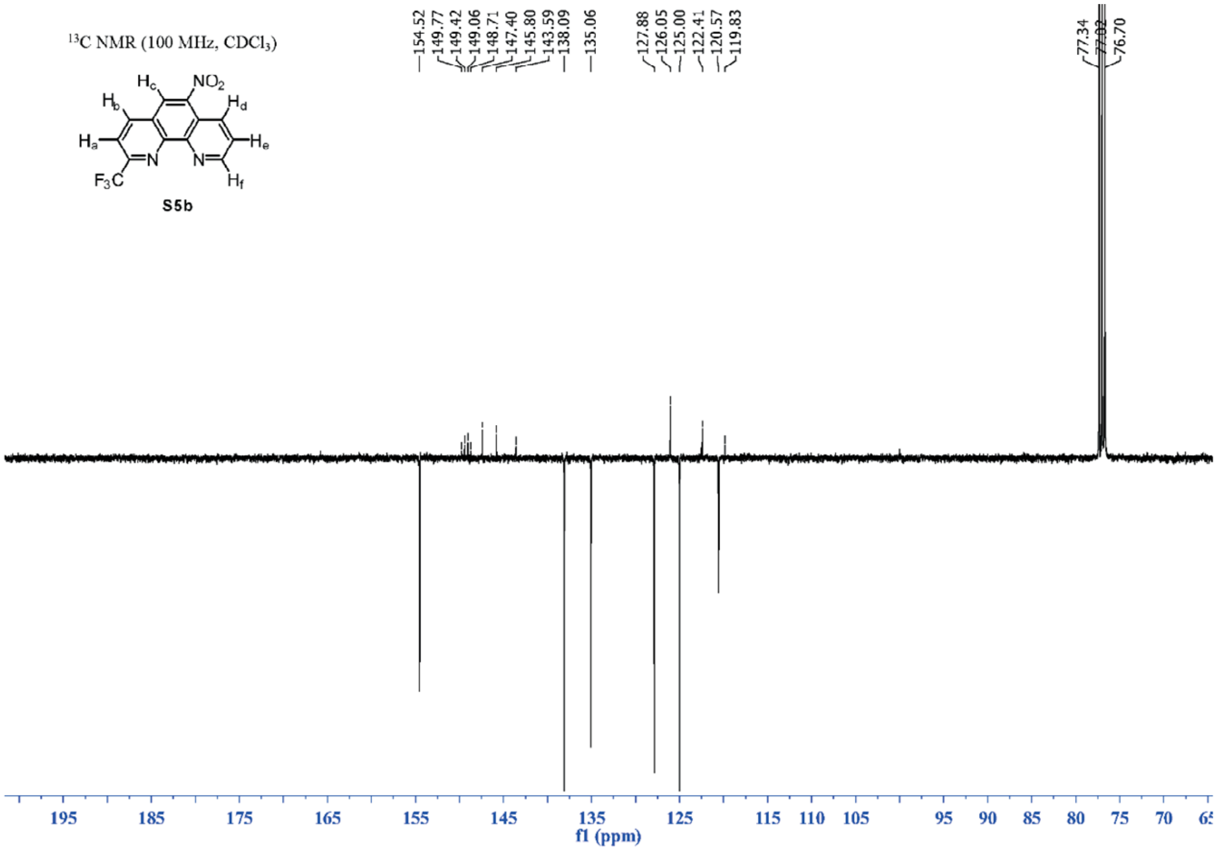

-67.00
19F NMR (377 MHz, CDCl3)
Hd
NO2
Hc
He
Hb
Hf
N
N
Ha
CF3
S5a
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

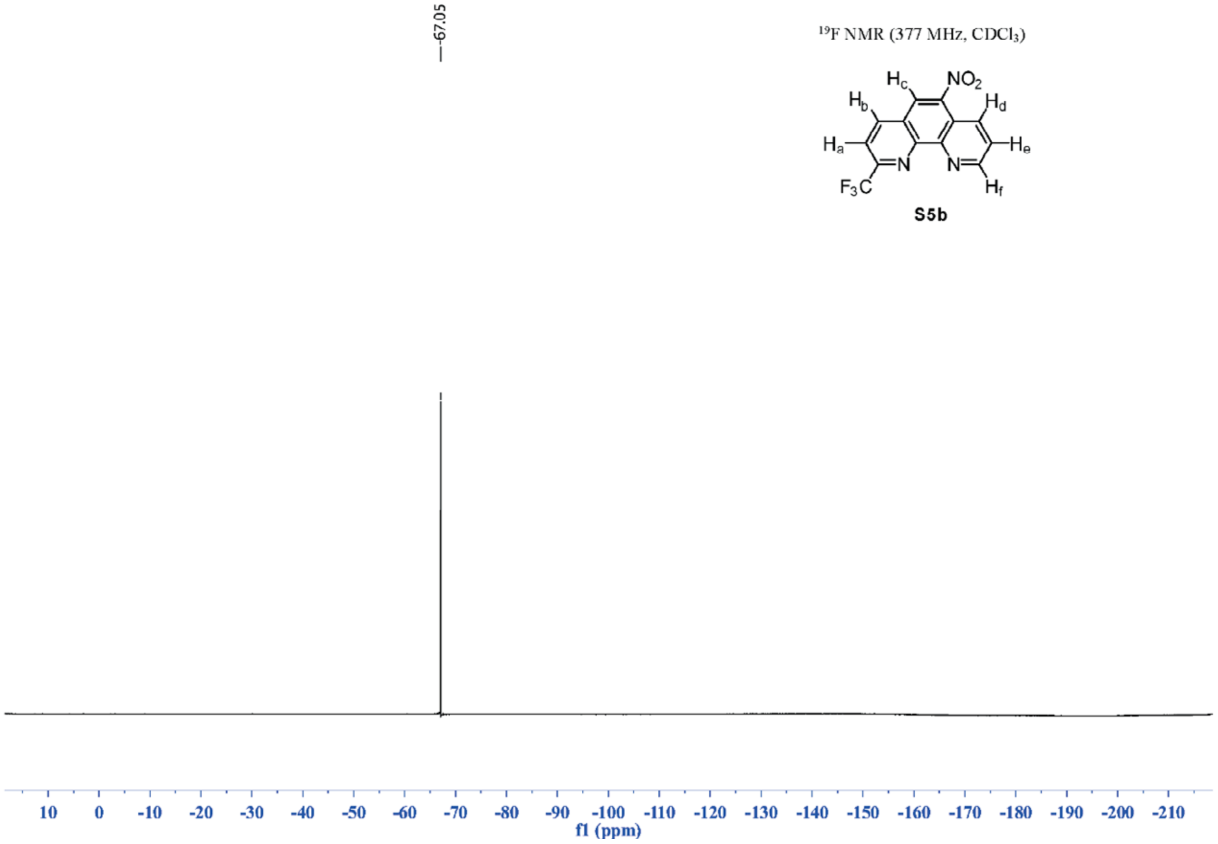


^{1}H NMR (400 MHz, CDCl$_3$)




NOESY
S5b
NO2
F3C
N
Ha
Hb
Hc
Hd
He
Hf
NOE
ppm
7.6
7.8
8.0
8.2
8.4
8.6
8.8
9.0
9.2
9.4
9.6
9.8


13C NMR (100 MHz, CDCl3)
Hc
NO2
Hb
Hd
Ha
He
F3C
N
N
Hf
S5b
154.52
149.77
149.42
149.06
148.71
147.40
145.80
143.59
138.09
135.06
127.88
126.05
125.00
122.41
120.57
119.83
77.34
77.02
76.70
195
185
175
165
155
145
135
125
115
110
105
95
90
85
80
75
70
65
f1 (ppm)


-67.05
19F NMR (377 MHz, CDCl3)
Hc
NO2
Hb
Hd
Ha
He
F3C
N
N
Hf
S5b
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)